ACS Chemistry for Life®

255TH AMERICAN CHEMICAL SOCIETY
NATIONAL MEETING AND EXPOSITION

Nexus of

FOOD ENERGY & WATER.

NEW ORLEANS
LOUISIANA

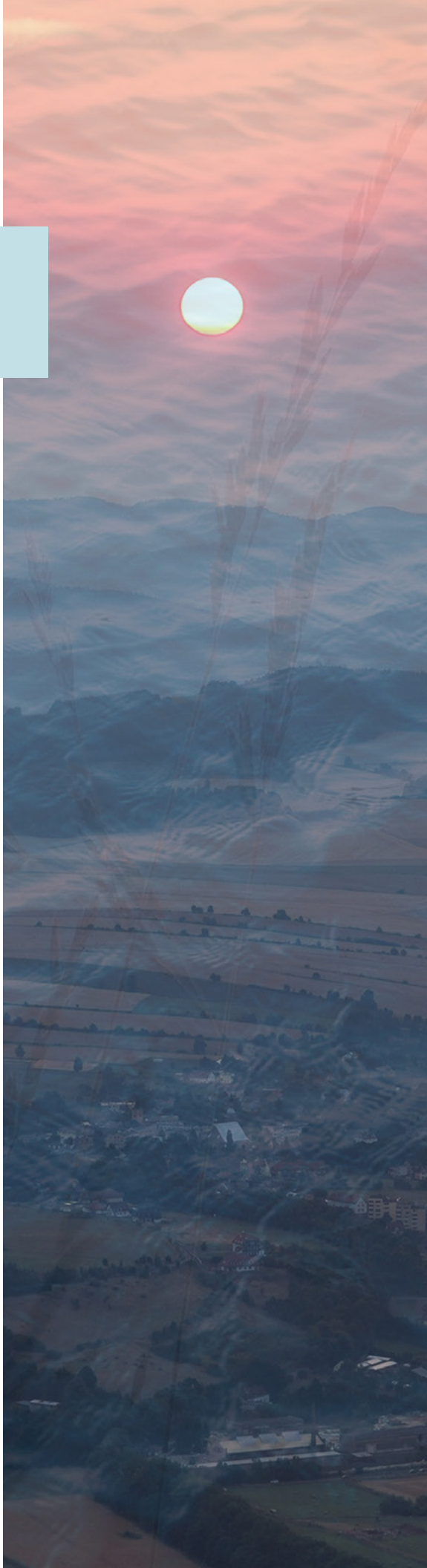
MARCH 18 – 22 2018

PROGRAM BOOK

ACS Chemistry for Life®

Visit the ACS Exposition & Career Fair!

Halls B2/C, Ernest N. Morial Convention Center



Join us for the Welcome Reception & Poster Sessions

Sunday, March 18
6:00 PM – 8:30 PM

Come back on Monday and Tuesday to continue visiting over 250 companies!

- Learn more about ACS benefits, products, services and merchandise at the ACS Booth
- Attend exhibitor workshops and demonstrations
- Network at the recharge lounge
- Meet recruiters from top companies at the Career Fair

This and much more is all happening on the newly designed ACS Expo Floor!

Monday, March 19
9:00 AM – 5:00 PM

Tuesday, March 20
9:00 AM – 5:00 PM

Caffeinate and communicate during coffee breaks!

Monday, March 19
1:00 PM – 3:00 PM

Tuesday, March 20
3:00 PM – 5:00 PM

255TH AMERICAN CHEMICAL SOCIETY
NATIONAL MEETING & EXPOSITION

TABLE OF CONTENTS

SYMPOSIUM

NANO IN FOOD, ENERGY, & WATER

MONDAY, MARCH 19, 1 PM

ROOM 215 | ERNEST N. MORIAL CONVENTION CENTER

SPEAKERS

JILLIAN M. BURIAK
University of Alberta

YURY GOGOTSI
Drexel University

YI CUI
Stanford University

BRIAN A. KORGEL
University of Texas at Austin

DELIA J. MILLIRON
University of Texas at Austin

HARRY ATWATER
California Institute of Technology

ACS NANO | ACS Photonics | CM Chemistry of Materials | NANO LETTERS

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The American Chemical Society is a self-governed individual membership organization of members at all degree levels and in all fields of chemistry. The Society provides a broad range of opportunities for peer interaction and career development, regardless of professional or scientific interests. The programs and activities conducted by ACS today are the products of a tradition of excellence in meeting member needs that dates from the Society's founding in 1876.

This Program Book is published by the American Chemical Society as a service to its meeting attendees. Information contained herein is subject to change without notice. While every effort is made to ensure accuracy, ACS makes no warranties, expressed or implied, related to the information. For the official technical program for the 255th National Meeting & Exposition, refer to www.acs.org/nationalmeeting.

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Fax: 202-872-4615
Email: help@acs.org
Website: www.acs.org

A WELCOME LETTER FROM ACS PRESIDENT, PETER K. DORHOUT

Welcome to New Orleans, Louisiana, and the site of the 255th ACS National Meeting. It is my pleasure to welcome all of you to The Big Easy.

With thousands of presenters and attendees, and hundreds of expo booths, there are tremendous opportunities to share your science, network, and catch up with colleagues. There are noteworthy technical symposia organized under the theme of this meeting: the Nexus of Food, Energy & Water.

On Sunday morning, I hope you are able to attend the Presidential symposium on Water, Water Everywhere But not a Drop to Drink, where we hear from renowned scientists discussing methods of preserving, protecting and delivering clean water. Later that afternoon, join your colleagues at another Presidential symposium exploring Science Cafes and Engaging the Public. Science cafes are an exceptional method of delving into a scientific issue within a community in a fun and lively manner. Speakers will discuss best practices and tips for initiating Science Cafes in your communities, with a reception to follow (both symposia are in the Hilton New Orleans Riverside, Grand Salon B, Sections 9-12).

On Monday at noon, join your colleagues at the ACS Board of Directors Regular Session where our featured speaker, Lisa Balbes, will discuss Nontraditional Careers for Chemists: Thinking Outside the Beaker (Ernest N. Morial Convention Center, Great Hall A). Later that afternoon, Emily Cranston from McMaster University will present the Kavli Foundation Emerging Leader in Chemistry Lecture on Transforming nanocellulose into sustainable products through surface engineering. Following her presentation, Angela Belcher of the Massachusetts Institute of Technology will give the Fred Kavli Innovations in Chemistry Lecture on Giving new life to materials for energy, the environment and medicine (both lectures are in the Ernest N. Morial Convention Center, Great Hall A).

On Tuesday evening, we recognize the outstanding accomplishments of our ACS National Award winners. If you are unable to attend the full program, please note that anyone can attend the Priestley Medal address, this year honoring Geraldine Richmond (New Orleans Marriott, Grand Ballroom).

Many career development programs for undergraduate and graduate students, postdocs, and chemical professionals will be offered. For job seekers and employers, the career fair will provide opportunities for on-site interviews, one-on-one career assistance, and career-related workshops. The exposition will feature several hundred companies showcasing services, instruments, books, and lab equipment in more than 300 booths.

As with any gathering of professional colleagues, we owe it to ourselves to be mindful of safety. Please become familiar with the emergency procedures in your hotel, your meeting rooms, and in other gatherings, and be aware of your surroundings. If you observe unsafe practices or situations, please say something to help our members stay safe. I love safety!

My personal thanks go to our hosts at the Louisiana Section, and the divisional program chairs and symposium chairs responsible for organizing the technical sessions. I know this will be a tremendously successful meeting, and I thank you all for your contributions.

Peter K. Dorhout
ACS President

Peter K. Dorhout, Ph.D.
ACS President

PRESIDENTIAL SYMPOSIA AND EVENTS

SPONSORED AND RECOMMENDED BY THE ACS PRESIDENT

SATURDAY, MARCH 17, 2018

Presidential Outreach Event: Exploring Our World Through Chemistry
Cosponsored by CCA
Lyons Recreation Center
624 Louisiana Ave, New Orleans
10:00 AM - 1:00 PM

SUNDAY, MARCH 18, 2018

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clear Water
Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS,CHED, COLL, CTA, ENVR, GEOC, INOR, I&EC, MPPG, SCHB & YCC
Hilton New Orleans Riverside | Grand Salon B
Sections 9/12 | First Floor
8:30 AM - 10:50 AM

Science Cafes and Engaging the Public: Techniques for Hosting Successful Events
Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, INOR, I&EC, MPPG, SCHB & YCC
Hilton New Orleans Riverside
Grand Salon B | Sections 9/12 | First Floor
1:30 PM - 5:20 PM

Nexus of Food, Energy, & Water
Sponsored by MPPG and Cosponsored by PRES
Ernest N. Morial Convention Center
Great Hall A First Floor
3:00 PM - 6:00 PM

MONDAY, MARCH 20, 2018

Community Sharing of Chemical Safety Data: Yes, No, Maybe?
Sponsored by CINF and Cosponsored by PRES CA & CHAS
New Orleans Marriott Convention Center
River Bend 1 | Second Floor
8:20 AM - 12:20 PM

TUESDAY, MARCH 20, 2018

GSSPC: Finding Our Place at the Bottom: A Symposium in Memory of Richard Feynman
Sponsored by CHED and Cosponsored by PRES, ANYL, COLL, ENVR, INOR & PMSE
New Orleans Marriott Convention Center
Blaine Kern C | First Floor
1:30 PM - 4:55 PM

OTHER SYMPOSIA RECOMMENDED BY THE ACS PRESIDENT

SUNDAY, MARCH 18, 2018

Science of Sexual Harassment
Sponsored by WCC and Cosponsored by PRES, C&EN, PROF & YCC
Hilton New Orleans Riverside | Grand Salon C
Section 13 | First Floor
9:00 AM - 4:50 PM

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF and Cosponsored by PRES, ANYL, BIOT, BIOL, CHED, CMA, COLL, COMP, CWD, ENVR, INOR,MEDI, ORGN, PHYS, POLY, PMSE, WCC &YCC
Hilton New Orleans Riverside
Grand Salon D Section 22 | First Floor
9:00 AM - 4:50 PM

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Scholar Research Symposium
CHED, DAC, MPPG & Louisiana Local Section
Hilton New Orleans Riverside | Grand Salon D
Section 24 | First Floor
1:00 PM - 4:40 PM

MONDAY, MARCH 19, 2018

State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry
Sponsored by CHED and Cosponsored by PRES
New Orleans Marriott Convention Center |
Blaine Kern E | First Floor
8:30 AM - 3:50 PM

Excellence in Graduate Polymer Research
Sponsored POLY and Cosponsored by PRES, PROF, SOCED & YCC
New Orleans Marriott Canal Street | Studio 5
Second Floor
8:00 AM - 4:40 PM

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST and Cosponsored by PRES, AGFD, CHED, DAC, MPPG & Louisiana Local Section
Hilton New Orleans Riverside | Grand Salon D
Section 24 | First Floor
8:30 AM - 5:40 PM

Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web
Sponsored by CINF and Cosponsored by PRES & HIST
New Orleans Marriott Convention Center | River Bend 1| Second Floor
1:15 PM - 5:05 PM

Science of Sexual Harassment
Sponsored by WCC and Cosponsored by PRES, C&EN, PROF & YCC
Hilton New Orleans Riverside | Grand Salon C
Section 13 | First Floor
3:00 PM - 5:00 PM

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF and Cosponsored by PRES, ANYL, BIOT, BIOL, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, POLY, PMSE, WCC &YCC
Hilton New Orleans Riverside | Grand Salon D
Section 22| First Floor
3:00 PM - 5:00 PM

TUESDAY, MARCH 20, 2018

Excellence in Graduate Polymer Research
Sponsored POLY and Cosponsored by PRES, PROF, SOCED & YCC
New Orleans Marriott Canal Street | Studio 5
Second Floor
8:00 AM - 5:40 PM
Ernest N. Morial Convention Center | Hall D
First Floor
6:00 PM - 8:00 PM

Water Supply Safety
Sponsored by CHAS and Cosponsored by PRES, CCS & ENVR
Hilton New Orleans Riverside | Grand Salon D
Section 21
First Floor
9:00 AM - 11:30 AM

Science Cafés and Engaging the Public: Techniques for Hosting Successful Events
Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, INOR, I&EC, MPPG, SCHB & YCC
Hilton New Orleans Riverside
Grand Salon B | Sections 9/12 | First Floor
1:30 PM - 5:20 PM

WELCOME MESSAGE FROM JERALD L. SCHNOOR, NEW ORLEANS THEMATIC CHAIR

The 255th ACS National Meeting will showcase topics on the *Nexus of Food, Energy and Water.* Food, energy and water are vital for life and for advancing the human condition. Yet, poverty, increasing population and burgeoning consumption cause acute and chronic shortages of these staples throughout the world. Inextricably linked are food, energy and water. At the nexus of energy and water, we understand that one cannot obtain freshwater without an investment in energy, and vice versa. It is also difficult for agriculture to grow more food without abundant water for irrigation. Still, cheap energy is key to obtaining both food and water, but the constraints of climate change make low-carbon energy a necessity. As scientists and engineers, we understand that chemistry can play a huge role in achieving food, energy and water security. For example, novel chemical materials can help to develop solar energy cells more cheaply, membranes for separation of water from brines, and new pesticides and fertilizers, which conserve the diversity of ecosystems, soil and water Thematic Program Chair quality. At the 255th ACS National Meeting, we will explore green chemistry, nanoscience, biofuels and many other sustainable solutions at the nexus of all three — food, energy and water.

The Opening Session on Sunday afternoon, March 18, will inaugurate the theme, *Nexus of Food, Energy and Water: Adapting to Future Challenges,* with five guest lecturers:

- Professor Mark Jacobson (Stanford University) will lead with a solution, "Transitioning World Energy for All Purposes to Stable Electricity Powered by 100% Wind, Water, and Sunlight"
- Professor Yun Hang Hu (Michigan Technological University) will present an overview of "Advanced Materials and Processes for Energy and Water"
- Professor Pratim Biswas (Washington University) will discuss his lab's innovative material science solutions, "Nanoparticle Technology Enabling Smart Agriculture Solutions: Nexus of Food and Environment"
- Professor David Dzombak (Carnegie Mellon University) will describe water problems with the energy revolution in shale gas, "Hydraulic Fracturing and Drinking Water Resources"
- Professor Amy Childress (University of Southern California) will speak at the water/energy nexus, "Integrating Systems of Water Reuse and Desalination: More Water, Less Energy"

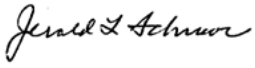
On Monday, March 19, Professor Angie Belcher of the Massachusetts Institute of Technology will deliver the Fred Kavli Innovations in Chemistry Lecture. Professor Belcher's fascinating work using nature and biomaterials to grow batteries (novel energy systems) will be the foundation of her remarks. The session will be coupled with the Kavli Foundation Emerging Leader in Chemistry Lecture, and you will not want to miss it.

An exceptional technical program constructed by the ACS divisions includes both topical sessions and symposia honoring the winners of ACS awards. Nineteen divisions offer 63 symposia on the theme. In addition, our Multidisciplinary Planning Group MPPG and partner divisions add multiple half and full day symposia focused on the theme, Nexus of Food, Energy and Water, such as:

- Food vs. Fuels (ENFL/AGFD/ENVR): Ms. Lisa Houston (Process Analytics, PAC LP).
- Water in Foods Symposium in honor of Louise Slade & Harry Levine (AGFD): Dr. John Finley (LSU) and Dr. Emily Maung-Douglass (LSU).
- Plant Omics (MPPG): Professor Leslie Hicks (UNC).
- Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present (HIST): Professor Mary Virginia Orna (CNR) and Professor Alvin Bopp (SUNO).
- Contaminants in Water Sources Impacted by FEW Systems: Emerging Challenges & Opportunities (ENVR): Professor Gregory LeFevre (UIowa).

The program for the meeting and other information is available online at the website for the New Orleans 2018 National ACS meeting, www.acs.org/nationalmeeting. The final day of the meeting, Thursday, March 22, is fittingly the *United Nations World Water Day,* and we have several technical sessions on producing abundant and clean freshwater for people.

I am very grateful to the theme session chairs for their efforts, the program chairs of a broad range of 19 divisions, and the ACS staff for their continuous aid in developing the *Nexus of Food, Energy and Water* theme. I look forward to seeing you in New Orleans.



Jerald L. Schnoor
Thematic Program Chair

OPENING SESSION & WELCOME RECEPTION

Sunday, March 18, 2018

Opening Session

3:00 PM–6:00 PM

Great Hall A, Ernest N. Morial Convention Center

Kick off the National Meeting & Exposition in New Orleans with the Opening Session on *Nexus of Food, Energy & Water: Adapting to Future Challenges.*

Professor Mark Jacobson (Stanford University) will lead with a solution, "Transitioning World Energy for All Purposes to Stable Electricity Powered by 100% Wind, Water, and Sunlight"

Professor Yun Hang Hu (Michigan Technological University) will present an overview of "Advanced Materials and Processes for Energy and Water"

Professor Pratim Biswas (Washington University) will discuss his lab's innovative material science solutions, "Nanoparticle Technology Enabling Smart Agriculture Solutions: Nexus of Food and Environment"

Professor David Dzombak (Carnegie Mellon University) will describe water problems with the energy revolution in shale gas, "Hydraulic Fracturing and Drinking Water Resources"

Professor Amy Childress (University of Southern California) will speak at the water/energy nexus, "Integrating Systems of Water Reuse and Desalination: More Water, Less Energy"

Welcome Reception

6:00 PM–8:30 PM

Halls B2/C, Ernest N. Morial Convention Center

Join us Monday, March 19 for the Kavli Lecture Series

THE KAVLI FOUNDATION

4:00 PM

The Kavli Foundation Emerging Leader in Chemistry Lecture

Dr. Emily Cranston (McMaster University in Canada) describes recent advances in hybrid cellulose nanocrystal (CNC) material development and show applications in emulsions/emulsion polymerization, injectable hydrogels and cross-linked aerogels. This new understanding can be used to extend food, cosmetic, paint and adhesive products, encapsulation technologies, tissue engineering scaffolds, and water purification and energy storage devices.

5:15 PM

The Fred Kavli Innovations in Chemistry Lecture

Prof. Angela Belcher (Massachusetts Institute of Technology) speaks on her fascinating work using nature and biomaterials as inspiration to design biological hybrid multidimensional materials. This talk will address conditions under which organisms first evolved to make materials and scientific approaches to move beyond naturally evolved materials to genetically imprint advanced technologies with examples in lithium and sodium ion batteries, lithium-air batteries, environmental clean-up and ovarian cancer imaging and treatment.

ACS Chemistry for Life®

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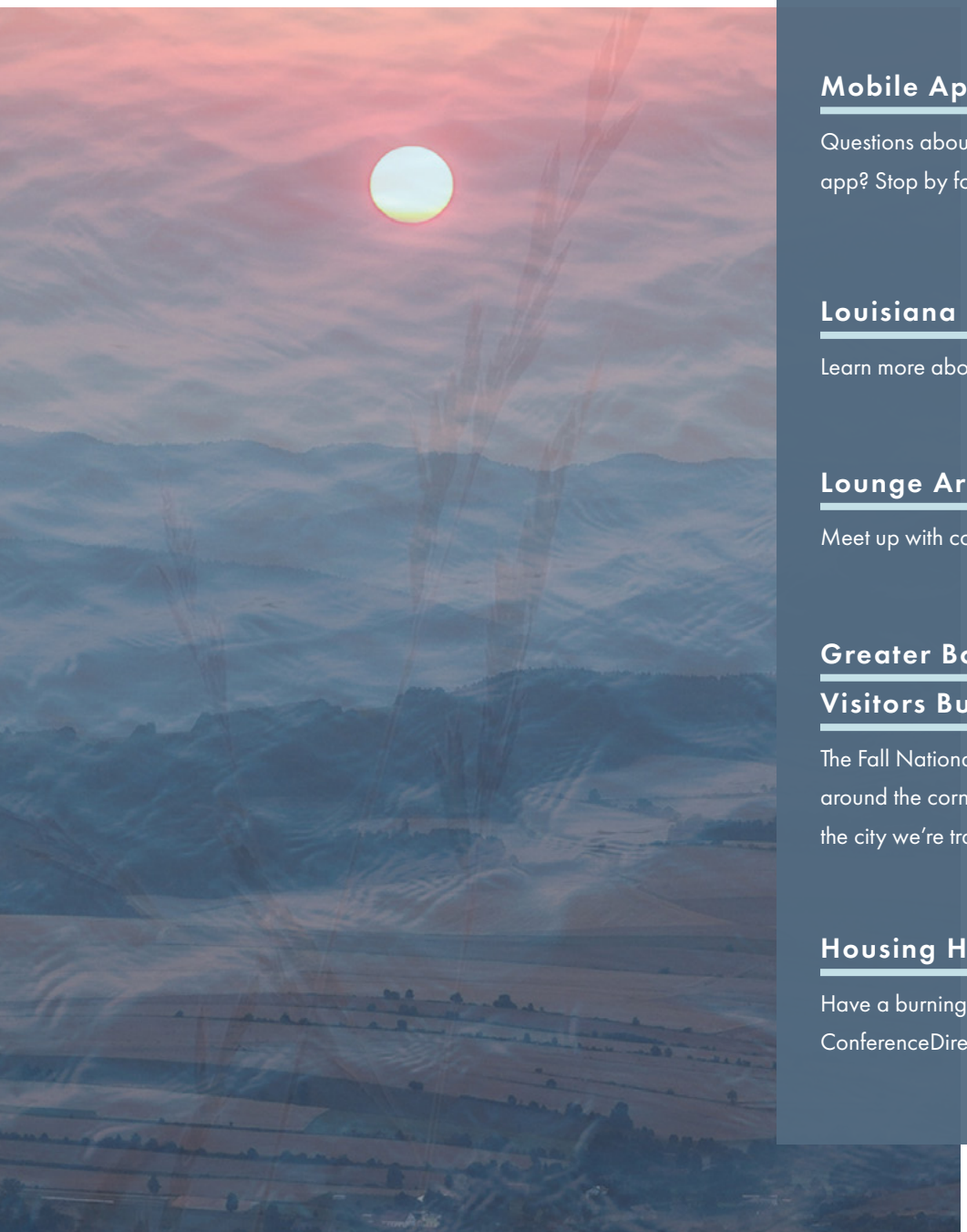
Lounge Room, Ernest E. Morial Convention Center

Hours

Sunday, 7:30 AM – 5:00 PM
Monday, 7:30 AM – 5:00 PM
Tuesday, 7:30 AM – 5:00 PM
Wednesday, 7:30 AM – 4:00 PM
Thursday, 7:30 AM - 1:00 PM



What Element Are You?

Take the quiz at www.acs.org/ElementQuiz. Come by the Hub to pick up your element free gift!

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Pick up gifts for yourself or a chemist in your life!

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Louisiana Local Section

Learn more about the ACS Local Section in our host state!

Lounge Area with Charging Spots

Meet up with colleagues and recharge your devices.

Greater Boston Convention & Visitors Bureau

The Fall National Meeting & Exposition in August is around the corner. Chat with locals to hear more about the city we're traveling to.

Housing Help Desk

Have a burning question about your hotel reservation? ConferenceDirect is here to help.

JOIN US FOR THE ACS BOARD OF DIRECTORS REGULAR SESSION

Sunday, March 18, 2018 | 12:00 PM –1:00 PM
New Orleans Ernest N. Morial Convention Center | Great Hall A

"Nontraditional Careers for Chemists: Thinking Outside the Beaker"

A chemistry background prepares you for much more than a laboratory career. The broad science education, analytical thinking, research methods, and other skills learned are of value to a wide variety of employers, and essential for a plethora of positions. By understanding your own personal values and interests, you can make informed decisions about what career paths to explore, and identify positions that match your needs. This talk will provide a broad overview of nontraditional careers for chemists, such as chemical information, patent work, technical writing, education, human resources, sales and marketing, and much more. We will discuss typical tasks, education or training requirements, and personal characteristics that will also be provided.

Featured Speaker
Lisa M. Balbes, Ph.D.
Balbes Consultants, LLC

Dr. Lisa M. Balbes has been an American Chemical Society volunteer career consultant since 1993, providing career management advice and information to literally thousands of scientists. She is the author of "Nontraditional Careers for Chemists: New Formulas in Chemistry", published by Oxford University Press, an ACS certified master workshop facilitator, and an internationally invited speaker on various career topics. She earned her Ph.D. in chemistry from the University of North Carolina at Chapel Hill, and her undergraduate degrees in chemistry and psychology from Washington University in St Louis.

Doors open at 11:45 AM
Sandwiches and soft drinks available while supplies last.

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A WELCOME LETTER FROM MAYOR MITCHELL J. LANDRIEU

City Of New Orleans

Welcome!

As Mayor of New Orleans, it is my pleasure to welcome the American Chemical Society. Thank you for choosing to celebrate your annual national meeting in New Orleans.

You will experience the warm hospitality and unique culture that New Orleans has to offer. I am certain that New Orleans will serve as the perfect destination for the meeting and provide the best opportunities for the group. While you are here, take some time to relax and explore the City. Dine in our incomparable restaurants; enjoy some of the great music we have to offer, tour historic neighborhoods like the French Quarter and Treme, and shop in our antique and specialty shops throughout New Orleans, including the bustling Magazine Street corridor. It is my hope that your stay will be memorable and that you leave with new knowledge and relationships.

I extend my best wishes to the American Chemical Society, as well as those traveling to partake in the meeting. I want to thank you again for choosing New Orleans.

Sincerely,

Mitchell J. Landrieu, Mayor
City of New Orleans

A WELCOME LETTER FROM THE NEW ORLEANS CONVENTION & VISITORS BUREAU

Dear attendees of the American Chemical Society,

It is my pleasure to welcome the American Chemical Society (ACS) to New Orleans for the ACS National Meeting & Expo. It is a great honor to host you all in one of America's most historic and culturally rich destinations...a city that visitors have loved for centuries.

New Orleans has always been a destination that welcomes all and there has never been a better time to experience the Crescent City. Thanks to the dedication of locals and visitors alike, New Orleans is experiencing a true economic and cultural renaissance. As we prepare for our tricentennial celebration in 2018, the city is bustling with progress and innovation. From the development of a new world class airport opening in 2019, a re-energizing billion-dollar project along the riverfront, to small independent businesses in the eclectic, historic neighborhoods of Tremé, Bywater, Magazine Street and Faubourg Marigny, business and culture are booming.

While you are here, you owe it to your soul to immerse yourself in our rich culture and enjoy all that our beautiful, sensory and authentic city has to offer. I'm certain you will see that New Orleans is the perfect backdrop for your historic anniversary meeting. Be sure to explore our 1,500+ restaurants from the traditional pillars of New Orleans dining celebrated throughout the years, to the emergent new chefs offering stunningly innovative international cuisine and world-class fusions of culinary traditions... all here in the most award-winning city for food per capita in the world. No place has a better combination of elegant fine dining, food under ten dollars and the greatest mixology found anywhere on Earth from morning till long past midnight, while the riffs of jazz music fill your ears everywhere you stroll. On behalf of the entire hospitality community – chefs, street performers, musicians, bellmen, artists, actors, writers and housekeepers – welcome to New Orleans. We are thrilled to host this event and are happy to be your "source for exploration" for the next few days. We hope you enjoy your stay and return often to our wonderful city.

Best Regards,

Stephen

Stephen Perry
President and CEO
New Orleans Convention & Visitors Bureau

acs.axial.com/new-orleans

Join us in welcoming new journals to the ACS Publications family

Meet the Editors

Kirk S. Schanze
University of Texas, San Antonio

Gerald J. Meyer
University of North Carolina at Chapel Hill

T. Randall Lee
University of Houston

Shu Wang
Institute of Chemistry, Chinese Academy of Sciences

Monday, March 19, 2018

10AM, ACS Booth Theater, Exhibits Hall
Refreshments provided

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ACS APPLIED ENERGY MATERIALS

ACS APPLIED NANO MATERIALS

ACS Pharmacology & Translational Science

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Silver Level

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GENERAL MEETING INFORMATION

Welcome to New Orleans, home of the 255th National Meeting of the American Chemical Society. Over the next five days, as you explore the Nexus of Food, Energy & Water, you will have opportunities to connect with thousands of chemical professionals from around the globe to share ideas and examine emerging scientific and technical knowledge in the field of chemistry. The meeting agenda includes educational offerings complemented by social events and networking opportunities.

Your meeting registration gives you entry to a range of programming activities, including:

- Award Presentations
- Exposition Hall and Career Fair
- Invited Symposia
- Scientific and Poster Sessions
- Special Lectures, Workshops, and Events

Meeting activities will take place in the Ernest N. Morial Convention Center and nearby hotels. All meeting venues have an ACS Operations Office with available staff to answer your questions.

Program Book

A limited number of Program Books are available for sale if you did not purchase one when you registered. You can buy the book in the Attendee Registration Office located in Lobby A of the Ernest N. Morial Convention Center, Rivergate Ballroom. The cost is $20, payable by credit card, debit card, or check.

We encourage meeting attendees to download the ACS Meetings & Events Mobile App or access the Online Planner from the ACS website. The ACS Meetings & Events Mobile App is the official final meeting program and will provide quick access to the full technical program along with special features so you can easily build your schedule.

ACS Operations Offices

- **Embassy Suites New Orleans, *Fountainbleu 3***
  504-378-4046
- **Ernest N. Morial Convention Center, *Rivergate Ballroom***
  504-670-6704
- **Hampton Inn & Suites Convention Center, *Dauphine I Meeting Room***
  504-566-9990 Ext. 7906
- **Hilton Garden Inn Convention Center, *Library***
  504-310-1149
- **Hilton New Orleans Riverside, *Magazine***
  504-586-4613
- **InterContinental New Orleans, *Acadian II***
  504-585-7847
- **Le Meridien New Orleans, *Salon 4***
  504-525-9444 Ext. 4872
- **Loews New Orleans Hotel, *Guest Room 1121***
  504-595-5362
- **New Orleans Marriott Canal Street, *Bonaparte***
  504-553-5678
- **New Orleans Marriott Convention Center, *Delta Queen***
  504-613-2397
- **Renaissance New Orleans Art Hotel, *Blue Dog***
  504-613-2357

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  504-553-5665
- **Governance Office:**
  Hilton New Orleans Riverside, *Jackson*
  504-586-4608
- **Society Programs Office:**
  Hilton New Orleans Riverside, *Camp*
  504-586-4612

ACKNOWLEDGEMENTS

ACS Divisions and Committees are grateful for the financial donations and other contributions received throughout the year and specifically toward the National Meeting. Our accomplishments are due in large part to this support. All of us at ACS acknowledge our appreciation to the many government agencies, educational institutions, organizations, and companies listed below as well as the others omitted from this list because of printing deadlines.

Division of Agricultural and Food Chemistry

- Ajinomoto Co., Inc

Division of Analytical Chemistry

- Falcon Analytical
- Infometrix Inc
- Meinhard
- The College of the Holy Cross
- Thermo Fisher Scientific

Division of Biological Chemistry

- Journal of Biological Chemistry
- University of Massachsetts Amherst

Division of Business Development and Management

- CIEC

Division of Carbohydrate Chemistry

- Glen Research
- Shimadzu

Division of Cellulose and Renewable Materials

- Adolphe Merkle Institute, University of Fribourg
- Department of Sustainable Biomaterials: Virginia Tech
- Elsevier: Carbohydrate Polymers
- EPNOE
- MDPI Fibers
- School of Forest Resources: University of Maine
- The Center for Renewable Carbon: University of Tennessee

Division of Chemical Education

- ACS Green Chemistry Institute
- Anasazi Instruments
- Bruker BioSpin
- GCI: ACS Green Chemistry Institute
- I&EC Green Chemistry Subdivision
- IPEC
- JEOL
- Magritek
- Mestrelab

Division of Chemical Health and Safety

- AACT
- CANN

Division of Chemical Information

- Chemical Structure Association Trust
- Clarivate Analytics
- IUPAC for Committee on Publications and
- Cheminformatics Data Standards

Division of Colloid and Surface Chemistry

- Henan University
- King Abdullah University of Science and Technology

Division of Computers in Chemistry

- Gaussian Inc.
- OpenEye

Division of Environmental Chemistry

- AEESP
- Environmental Science & Technology
- Environmental Science & Technology Letters
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Division of Organic Chemistry

- Biogen
- Boehringer Ingelheim
- Chem (Cell Press)
- ChemComm/ChemSci
- ChemPhotoChem
- Denison University
- STREM
- Thieme

Division of Physical Chemistry

- U.S. Army Research Office

Division of Polymer Chemistry

- 3M

- Anton Paar USA, Inc.
- Arkema
- Bruker AXS, Inc.
- Cambridge Isotope
- Exxon
- ExxonMobil
- JEOL
- MR Resources
- New Era Enterprises
- NMR Service
- Pfizer
- POLY Industrial Advisory
- Board
- Rototec-Spintec
- Solvay
- The Dow Chemical Company
- Tosoh
- Wiley
- Wyatt Technology

Division of Polymeric Materials Science and Engineering

- ACS Brazil Chapter
- Anasys Instruments
- Applied Minerals, Inc.
- BASF
- Danimer Scientific
- Department of Chemistry & Biochemistry at Florida State University
- DuPont
- Eastman Chemical Company
- Elsevier
- ExxonMobil
- ExxonMobil Chemical Company
- IBM
- LG MMA
- MilliporeSigma
- North American Membrane Society
- NSF
- Ondax
- Tosoh Biosciences LLC
- Toyo Styrene Co., Ltd.
- University of Delaware Department of
- Materials Science & Engineering
- Wyatt Technology
- Zeon Corporation
- Zibo Zhangdian Oriental Chemical Co., Ltd.

Division of Small Chemical Businesses

- Saul Ewing LLP

Division of the History of Chemistry

- ACS Louisiana Local Section

Women Chemists Committee

- C&EN

Younger Chemists Committee

- C&EN

We Thank Our Volunteers for Their Dedication and Hard Work

ACS Volunteers contribute thousands of hours of service to create and implement programs that promote our science, benefit our members, and contribute to the development of our communities. Thanks to your contributions, the Society provides its over 150,000 members with:

- Powerful networks on the local, regional, and national levels
- Specialized technical information and research
- Expansive career enhancement materials
- Award winning publications
- Meetings & expositions that set industry standards for excellence.

ACS salutes the outstanding volunteer efforts that have contributed to the success of this year's national and regional meetings, including division chairs, national meeting program officers, regional meeting organizers and program chairs, symposium organizers, session and award presiders, short course and workshop instructors, career counselors, and all members of the Society's governance. To get involved, go to www.acs.org.

ACS VOLUNTEER/NATIONAL MEETING ATTENDEE CONDUCT POLICY

One of the key strengths of the ACS has been the enduring and varied contributions made by its thousands of dedicated volunteers.

Another unassailable strength of the ACS is its outstanding national meetings program. ACS national meetings are among the most respected scientific meetings in the world. ACS national meetings offer scientific professionals a legitimate platform to present, publish, discuss, and exhibit the most exciting research discoveries and technologies in chemistry and its related disciplines. Furthermore, ACS national meetings facilitate networking opportunities, career development and placement, and provide organizations with opportunities to exhibit products and services to targeted audiences.

The Society's Congressional Charter explicitly lists among its objectives "the improvement of the qualifications and usefulness of chemists through high standards of professional ethics, education and attainments...." The ACS expects its volunteers and national meeting attendees to display the highest qualities of personal and professional integrity in all aspects of their ACS related activities. Indeed, every chemical professional has obligations to the public, to volunteer and staff colleagues, and to science.

Accordingly, and to foster a positive environment built upon a foundation of trust, respect, open communications, and ethical behavior, the ACS Board of Directors has issued this Conduct Policy. It applies to ACS Volunteers, i.e., it applies to individuals conducting the business and affairs of the ACS without compensation for that conduct. It also applies to attendees at ACS national meetings. Volunteers and national meeting attendees should at all times abide by this Conduct Policy. Specifically:

- Volunteers should understand and support ACS's vision and mission.
- Volunteers and national meeting attendees should contribute to a collegial, inclusive, positive, and respectful environment for their fellow volunteers and attendees, as well as for other stakeholders, including national meeting vendors and ACS staff.
- Volunteers and national meeting attendees must avoid taking any inappropriate actions based on race, gender, age, religion, ethnicity, nationality, sexual orientation, gender expression, gender identity, marital status, political affiliation, presence of disabilities, or educational background. They should show consistent respect to colleagues, regardless of the level of their formal education and whether they are from industry, government or academia, or other scientific and engineering disciplines.
- Volunteers and national meeting attendees should interact with others in a cooperative and respectful manner. Volunteers and national meeting attendees should refrain from using insulting, harassing, or otherwise offensive language in their ACS interactions. Disruptive, harassing, or inappropriate behavior toward other volunteers, stakeholders, or staff is unacceptable. Personal boundaries set by others must be observed. Harassment of any kind, including but not limited to unwelcome sexual advances, requests for sexual favors, and other verbal or physical harassment will not be tolerated.
- Volunteers must obey all applicable laws and regulations of the relevant government authorities while acting on behalf of the ACS. Likewise, national meeting attendees must obey all applicable laws and regulations of the relevant government authorities while attending ACS national meetings. Volunteers and national meeting attendees alike should also ensure that they comply with all applicable safety guidelines relating to public chemistry demonstrations.
- Volunteers and national meeting attendees should only use ACS's trademarks, insignia, name, logos, and other intellectual property in compliance with ACS regulations and directives as may be issued from time to time.
- Violations of this Conduct Policy should be reported promptly to the ACS Secretary and General Counsel or to the Chair of the ACS Board of Directors. In cases of alleged persistent and/or serious violations of this Conduct Policy, the Board shall review the evidence and shall take such actions as may be appropriate, including but not limited to requiring volunteers to leave their volunteer position(s); precluding volunteers from serving in Society volunteer roles in the future; requiring national meeting attendees to leave the meeting; and, precluding meeting attendees from attending future ACS national meetings. ACS, through its Board of Directors, reserves the right to pursue additional measures as it may determine are appropriate.

ATTENDEE REGISTRATION

Registration Fees

Members

50-Year Member No Fee
ACS Affiliate $570
Emeritus or Retired $290
Graduate student $240
One-Day Registrant $290
Precollege Teacher $120
Undergraduate $120
Unemployed No Fee
Dues waiver required
Guest of Registrants* $50

*Restricted to a spouse or family member of an attendee having no affiliation with the field of chemical science and who is not eligible to become an ACS member. Only one guest registration is allowed per registered attendee, and the guest registration must be completed and paid by the registering attendee at time of original registration.

Join ACS Before You Register

Save up to $400 before you register! Visit the Membership Desk at registration in the Ernest N. Morial Convention Center, Lobby A, for more information and to complete your application.

Nonmember Fees

Chemical Scientist $995
Graduate student $475
One-day Registrant $570
Precollege teacher $120
Undergraduate $240

Expo-Only Admission

Adults Only $60
Students Only $30

Members of the Press

Registration is complimentary for credentialed members of the news media who are approved by the ACS Office of Communications. Press badges may be picked up in the ACS Press Center, Great Hall B/C, Ernest N. Morial Convention Center.

Attendee Registration

Ernest N. Morial Convention Center, Lobby A

Hours of Operation

Saturday, March 17, 3:00 PM to 6:00 PM
Sunday, March 18, 7:30 AM to 7:30 PM
Monday, March 19, 7:30 AM to 9:00 PM
Tuesday, March 20, 7:30 AM to 5:00 PM
Wednesday, March 21, 7:30 AM to 4:00 PM
Thursday, March 22, 7:30 AM to 1:00 PM

Satellite Registration Office:

Hilton New Orleans Riverside Hotel
First Floor Registration Center

Hours of Operation

Saturday, March 17, 3:00 PM to 6:00 PM
Sunday, March 18, 7:30 AM to 7:30 PM
Monday, March 19, 7:30 PM to 5:00 PM
Tuesday, March 20, 7:30 AM to 5:00 PM

What You Can Do at the Registration Desk

- Register for the meeting
- Pick up your badge & registration credentials (Persons who registered after February 5 & all international attendees.)
- Get a replacement badge
- Make changes to your registration (Bring your badge and or registration credentials with you for faster processing.)
- Pick up your Program Book (if purchased in advance.)
- Request a scooter
- Purchase a Program Book (limited number available)
- Purchase special & social event tickets

Reminders

- All attendees, including speakers and poster presenters, must register for the meeting to participate in the technical sessions.
- Remember to wear your badge at all times for admission to all official ACS sessions and events.

ACS Chemistry for Life®

255th ACS National Meeting & Exposition
March 18–22, 2018 • New Orleans, LA • #ACSNOLA

Shuttle Hours of Operation

SUNDAY, March 18
7:00 AM - 10:00 AM ..... 15 minute service
10:00 AM - 4:00 PM ..... 30 minute service
4:00 PM - 7:00 PM ..... 15 minute service
7:00 PM - 11:00 PM ..... 30 minute service

MONDAY, March 19
7:00 AM - 10:00 AM ..... 15 minute service
10:00 AM - 4:00 PM ..... 30 minute service
4:00 PM - 11:00 PM ..... 15 minute service

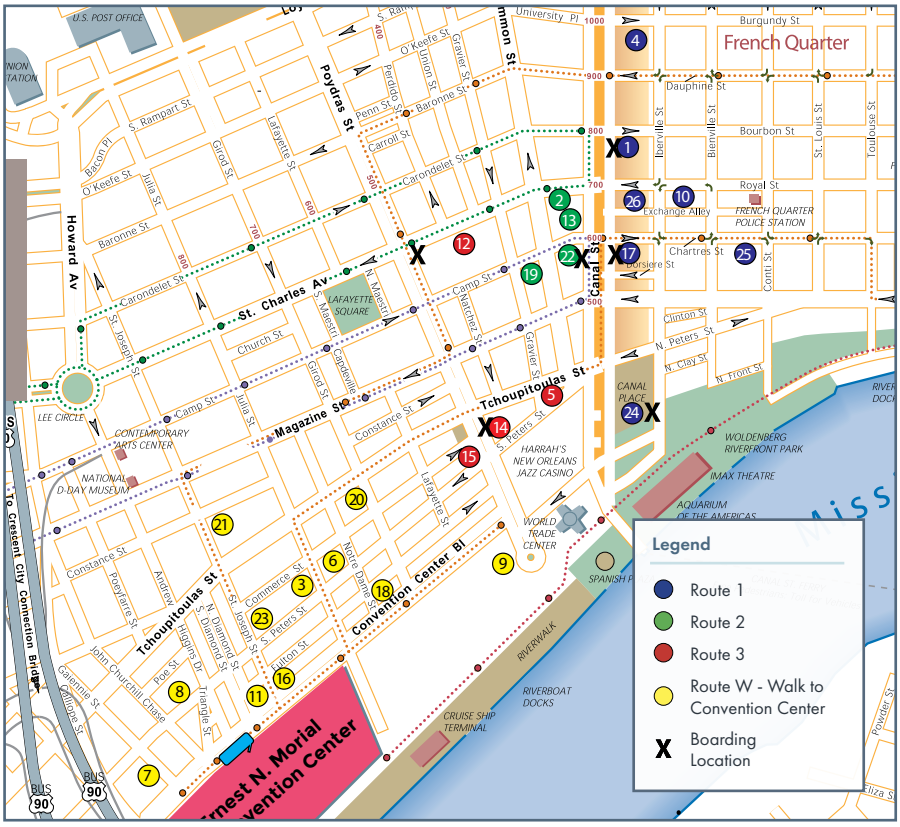
TUESDAY, March 20
7:00 AM - 10:00 AM ..... 15 minute service
10:00 AM - 4:00 PM ..... 30 minute service
4:00 PM - 11:00 PM ..... 15 minute service

WEDNESDAY, March 21
6:30 AM - 11:00 PM ..... 30 minute service

THURSDAY, March 22
7:00 AM - 6:00 PM ..... 60 minute service

Scan here to download a copy of this schedule onto your smart phone or device.

New Orleans Map



Key	Hotel	Route	Shuttle Boarding Location
1	Astor Crowne Plaza New Orleans French Quarter	1	Main Entrance - Canal St. & Bourbon St
2	Courtyard New Orleans Downtown Near the French Quarter	2	Walk to Sheraton New Orleans-Canal & Camp St
3	Courtyard New Orleans Downtown/Convention Center	W	Walk to Ernest N. Morial Convention Center
4	Courtyard New Orleans Downtown/Iberville	1	Walk to Astor Crowne Plaza - Canal St. & Bourbon St
5	DoubleTree by Hilton Hotel New Orleans	3	Walk to Le Meridien - Poydras St. & Tchoupitoulas St
6	Embassy Suites New Orleans	W	Walk to Ernest N. Morial Convention Center
7	Hampton Inn & Suites New Orleans-Convention Center	W	Walk to Ernest N. Morial Convention Center
8	Hilton Garden Inn New Orleans Convention Center	W	Walk to Ernest N. Morial Convention Center
9	Hilton New Orleans Riverside	W	Walk to Ernest N. Morial Convention Center
10	Hotel Monteleone New Orleans	1	Walk to Astor Crowne Plaza - Canal St. & Bourbon St
11	Hyatt Place New Orleans Convention Center	W	Walk to Ernest N. Morial Convention Center
12	InterContinental New Orleans	3	on Poydras St. & St. Charles
13	JW Marriott New Orleans	2	Walk to Sheraton New Orleans-Canal & Camp St
14	Le Meridien New Orleans	3	Main Entrance - Poydras St. & Tchoupitoulas St
15	Loews New Orleans Hotel	3	Walk to Le Meridien - Poydras St. & Tchoupitoulas St
16	New Orleans Downtown Marriott at the Convention Center	W	Walk to Ernest N. Morial Convention Center
17	New Orleans Marriott	1	Main Entrance - Canal St. & Chartres St
18	Omni Riverfront Hotel	W	Walk to Ernest N. Morial Convention Center
19	Omni Royal Crescent Hotel	2	Walk to Sheraton New Orleans-Canal & Camp St
20	Renaissance New Orleans Arts Hotel	W	Walk to Ernest N. Morial Convention Center
21	Residence Inn New Orleans Downtown	W	Walk to Ernest N. Morial Convention Center
22	Sheraton New Orleans	2	Main Entrance - Canal & Camp St
23	SpringHill Suites New Orleans Downtown/Convention Center	W	Walk to Ernest N. Morial Convention Center
24	The Westin New Orleans Canal Place	1	Iberville St. Entrance
25	W New Orleans - French Quarter	1	Walk to New Orleans Marriott - Canal St
26	Wyndham New Orleans - French Quarter	1	Walk to Astor Crowne Plaza - Canal St. & Bourbon St

For all shuttle and wheelchair assistance inquiries, please call:
1-866-439-8564

Shuttle service managed and operated by:

TMS
TRANSPORTATION MANAGEMENT SERVICES

Carbon Neutral Shuttles

#	LOCATION
1.	Astor Crowne Plaza New Orleans French Quarter
2.	Courtyard New Orleans Downtown Near the French Quarter
3.	Courtyard New Orleans Downtown/Convention Center
4.	Courtyard New Orleans Downtown/Iberville
5.	DoubleTree by Hilton Hotel New Orleans
6.	Embassy Suites New Orleans FLUO, NUCL
7.	Hampton Inn & Suites New Orleans-Convention Center CATL
8.	Hilton Garden Inn New Orleans Convention Center
9.	Hilton New Orleans Riverside BMGT, CHAS, CMA, CPRC, HIST, PRES, PROF, SCHB WCC, YCC
10.	Hotel Monteleone New Orleans
11.	Hyatt Place New Orleans Convention Center
12.	InterContinental New Orleans BIOT
13.	JW Marriott New Orleans POLY, PMSE
14.	Le Meridien
15.	Loews New Orleans Hotel CARB, CELL, I&EC
16.	New Orleans Downtown Marriott at the Convention Center CHED, CINF, COMP
17.	New Orleans Marriott
18.	Omni Riverfront Hotel
19.	Omni Royal Crescent Hotel
20.	Renaissance New Orleans Arts Hotel
21.	Residence Inn New Orleans Downtown
22.	Sheraton New Orleans
23.	SpringHill Suites New Orleans Downtown/Convention Center
24.	The Westin New Orleans Canal Place
25.	W New Orleans - French Quarter
26.	Wyndham New Orleans - French Quarter
27.	Ernest N. Morial Convention Center AGFD, ANYL, BIOL, CHAL, COLL, ENFL, ENVR, GEOC INOR, MEDI, MPPG, ORGN, PHYS, SOCED

ACCOMMODATIONS & TRAVELING TO MEETING SESSIONS

Accommodations

For attendees in need of housing, some official National Meeting hotels may still have rooms available. Visit the meeting website, www.acs.org/nationalmeeting, for the listing of official hotels.

ConferenceDirect is the official housing bureau for the National Meeting and ACS does not endorse booking hotel reservations through any other source. Attendee support of the official hotels allows ACS to use meeting space at a discount and to keep registration fees to a minimum. All attendees who make reservations through ConferenceDirect will receive complimentary internet access in their rooms.

Staff in the Housing Office will be available throughout the conference to assist you with last minute housing changes or needs. This office is in the ACS Resource Hub, located in the Ernest N. Morial Convention Center Lounge Room.

Getting to the Sessions

ACS Greeters:
Our greeters are positioned throughout the meeting venues and they can help you navigate the Program Book to find a particular session or room, and answer your meeting-related questions.

ACS Shuttle Bus:
The Ernest N. Morial Convention Center is located at 900 Convention Center Blvd. Many of the official hotels are in walking distance to the convention center. ACS will provide complimentary shuttle bus service between the Ernest N. Morial Convention Center and official hotels that are not in walking distance.

Parking:
The Ernest N. Morial Convention Center parking lot is directly across the street from the facility and the cost is $15.00 for the day.

Streetcar:
The Convention Center is a designated station along the Riverfront Streetcar route. The streetcar operates from 5:00 PM – 11:00 PM seven days a week.

Taxi Service:
The city of New Orleans has an extensive taxi service. Your hotel concierge can assist you with arranging taxi service.

Share Driving:
Lyft (lyft.com) and Uber (uber.com/ride) operate in New Orleans. Download the respective apps by visiting the websites.

HAPPENINGS AT THE ERNEST N. MORIAL CONVENTION CENTER

Points of Interest

- Attendee Registration, Lobby A, 504-670-6712
- Bus Shuttle Desk, Ticket Office, 504-670-6701
- Career Fair Information Center, Hall C, 504-670-6700
- Exhibitor Registration, Lobby B, 504-670-6717
- Finance Office, 504-670-6710
- Louisiana Local Section Booth, Lounge Room 504-670-6720
- Housing Assistance, Lounge Room, 504-670-6703
- Member Services, Lobby A, 504-670-6719
- Press Center, Great Hall B, 504-670-6721

Meetings

Sunday, March 18
- 3:00 PM to 6:00 PM: Opening Session, Ernest N. Morial Convention Center, Grand Hall A
- 6:00 PM to 8:30 PM: Welcome Reception in the Expo & Career Fair, Halls B2/C

Monday, March 19
- 4:00 PM to 6:30 PM: Kavli Lecture Series, Grand Hall A
- 8:00 PM to 10:00 PM: SciMix, Halls D & E

The UPS Store

The UPS Store, located in Lobby F, is both a self-service and full-service operation. A wide range of services are available, including digital printing, packing & shipping, notary services, and computer services. You can also copy and fax documents, purchase shipping materials and other supplies, and send & receive money via Western Union.

THINGS TO KNOW

ACS National Awards

The ACS National Awards recognize individual or team accomplishments in diverse fields of chemical science. This year's ACS Awards dinner will be held on the evening of Tuesday, March 20, at the New Orleans Marriott Hotel. Dinner begins at 7:30 PM, and the general meeting begins at 8:30 PM. Learn more about the awards dinner and the honorees at the meeting website, www.acs.org/nationalmeeting.

Camp ACS

Camp ACS is available to all meeting attendees free of charge from 7:00 AM to 6:00 PM, Sunday, March 18 through Thursday, March 22. If you wish for your child to participate in Camp ACS and you did not complete the registration by the March 2, deadline, go to the Convention Center ACS Operations Office located in the Rivergate Ballroom to speak with a staff person. Note: There is no guarantee the space is still available.

At Camp ACS, children two (and potty trained) to 16 years of age will participate in age-appropriate activities, including arts and crafts and active games, while you enjoy the meeting. For safety reasons, the location of Camp ACS is communicated to only attendees with enrolled children.

Emergencies During ACS Meeting Events

ACS has place detailed instructions inside each meeting room to be used if an emergency occurs during an ACS meeting event. These instructions revolve around following the established emergency guidelines of the facility where the emergency occurs. Report all emergencies to the nearest security guard or to any ACS Operations Office during the meeting.

If an emergency occurs outside an ACS event, contact the police or emergency assistance by dialing 911 or seeking assistance from the facility where the emergency has occurred.

Should a catastrophic event occur while the meeting is under way, follow safety and security instructions issued by the facility where you are located at the time of the event.

Lost-& Found

Lost items turned into an ACS Operations Office can be retrieved, with acceptable identification, during office operating hours. Items that are not returned by the close of the meeting will be turned over to the venue's security office.

Luggage & Coat Check

The luggage and coat check station is in the ACS Resource Hub located in the Convention Center Lounge Room.

Hours of operation are:

- Saturday, March 17: 3:00 PM to 6:30 PM
- Sunday, March 18: 7:30 AM to 7:30 PM
- Monday, March 19: 7:30 AM to 9:00 PM
- Tuesday, March 20: 7:30 AM to 7:00 PM
- Wednesday, March 21: 7:30 AM to 4:00 PM
- Thursday, March 22: 7:30 AM to 3:00 PM

Items left beyond the published hours of operation will be turned over to building security at the end of each day.

Mother's Room

For convenience and privacy, ACS has designated a room in the Ernest N. Morial Convention Center for nursing mothers. Please speak with a member of the Convention Center ACS Operations Office to gain access to the room.

Quiet Room

For those needing a space for quiet reflection while at the Ernest N. Morial Convention Center, you may go to the Information Booth or the ACS Operations at the Ernest N. Morial Convention to gain access to the room.

Sales Tax in New Orleans

The combined sales tax rate in New Orleans is 10%.

General Tipping Guidelines

Airport Porters & Bell Staff: $1.00/bag
Bartenders: 15-20%; Restaurant Wait Staff: 18-20%
Housekeeping Staff: $1-2/night

Wi-Fi Service

Enjoy free Wi-Fi service in the common areas of the Ernest N. Morial Convention Center.

MEETING POLICIES

ADA Compliance

ACS is dedicated to ensuring that no individual with a disability is excluded, denied services, segregated, or otherwise treated differently because of the absence of auxiliary aids and services identified in the Americans with Disabilities Act. If you have an emergency or need immediate assistance during the meeting, please contact any ACS Operations Office.

The Ernest N. Morial Convention Center is ADA compliant. It is equipped with service ramps to entrances and elevated areas; an array of passenger elevators, restroom facilities for the disabled; brailed instructions/directions at strategic locations throughout the building; and pay phones located at each level of the facility with (TDD) hearing-impaired functions.

Audio Taping, Photography & Videotaping

The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital recorders) or stream, upload or rebroadcast speakers or presentations is strictly prohibited at all official ACS meetings and events without express written consent from the ACS.

Badge & Badge Replacement

All attendees are required to wear their badges for all technical sessions, poster sessions, and all other official meeting events. Meeting badge holders are recyclable and biodegradable.

Please discard appropriately in the Badge Recycle bins positioned throughout the meeting venues.

If you misplace your badge and need a replacement please go to the Registration Office in Lobby A of the Ernest N. Morial Convention Center Rivergate Ballroom.

The badge replacement fees are:

- 1st replacement: free
- 2nd: $25 (cash/credit card)
- 3rd: $50 (cash/credit card)
- 4th & beyond: $100 each occurrence (cash/credit card)

Cancellation/Refund

Cancellation/refund requests received by February 27, 2018 will receive a refund, minus a $50 administrative fee. Requests received after February 27, 2018 are not eligible for a refund. Please direct questions regarding refunds to CDS at 508-743-0192 or 800-251-8629. Abstract USB drives and Program Books do not qualify for a refund.

Electronic Devices

As a courtesy to other meeting attendees, electronic devices must be operated in silent/ vibrate mode within technical or educational sessions. Cell phone conversations are not permitted in meeting rooms.

Literature & Product Distribution

Promotions, posters, and literature distribution by attendees, exhibitors, or other groups during the meeting must be done within their own contracted meeting space or exhibit booth and not in public meeting space, with the exception of designated marketing opportunities. Only ACS Operations Office staff is authorized to place any promotional items in public meeting space. Items left in violation of this policy will be removed and discarded.

Literature distribution at specific division tables is under the control of that division, and permission must be secured from the division before placing any items on its table.

Smoking

ACS policy prohibits smoking in all official meeting venue rooms during ACS functions. Additionally, as a reminder, the Convention Center and hotels are self-determined smoke-free environments at all times.

BE MINDFUL & AWARE

Everyday Safety Tips

- Be aware of your surroundings at all times.
- If someone or some place looks suspicious, report it and/or avoid it.
- Walk in open and well-lit areas at night.
- Travel in groups; do not be a loner, particularly in the evening.

Hotel Safety & Security

- Use the hotel safe deposit service or the in-room safe for valuables.
- If you leave items in your luggage, lock it when you leave the room.
- In crowded areas where you can be overheard, do not reveal your room number or discuss plans for leaving the hotel.

To & From Your Room

- If for any reason you are uncomfortable going to your room alone, ask a bellman or security officer to escort you and to check the room before you enter.
- Do not automatically open your door when someone knocks; use the door peephole to identify visitors before opening the door.
- Look into the elevator carefully before you enter. If you are uncertain of an occupant, wait for the next elevator.
- Look down the corridor carefully for suspicious activity before leaving the elevator.

To & From Events

- Remain alert at all times and be aware of your surroundings and the people you encounter.
- Remove your name badge when you are outside conference venues.

EXPOSITION AND CAREER FAIR HIGHLIGHTS

Exposition admission is complimentary for all national meeting registrants; however, you are required to wear your badge. Individuals who want to visit the exhibits without registering for the technical component of the national meeting can obtain an expo-only badge for $60. Students with school identification can obtain an expo-only badge for $30. Registration can be handled online, by mail, or in person at ACS attendee registration at the Ernest N. Morial Convention Center.

See What's New Inside the Exposition

Visit the ACS National Exposition at the Ernest N. Morial Convention Center, Halls B2/C, from Sunday, March 18, through Tuesday, March 20. Show hours are Sunday, 6:00 PM to 8:30 PM, and Monday and Tuesday, 9:00 AM to 5:00 PM.

Companies will display their most cutting edge services, instruments, computer hardware, scientific software, and a vast array of chromatographic, lab, and safety equipment. Technical personnel will give demonstrations, answer questions, and discuss your needs and interests. Join us at the ACS booth where ACS staff members will present the many benefits, services, products, and merchandise offered by ACS.

Exhibitor List & Floor Plan

Attendees can view a current list of exhibitors, videos, press releases, brochures, and flyers of participating exhibitors. Access the exposition at www.acs.org/nationalmeeting to learn more about exhibiting companies, plan your visit to the show floor, and download product information.

Exhibitor Workshops

Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the Convention Center. These workshops will hone your skills with specific tools and techniques and highlight innovative applications that will improve your productivity. Exhibitor workshop information is available at www.acs.org/nationalmeeting.

NEW: Recharge Lounge. Relax and recharge in our new networking lounge, located on the exhibit floor. Take a moment to chat with your fellow attendees while giving your devices an extra boost. Open during show hours.

Special Events in the Expo Hall

ACS Division Poster Sessions and Attendee Welcome Reception

Sunday, 6:00 PM – 8:30 PM

Afternoon Breaks

Monday, 1:00 PM – 3:00 PM
Tuesday, 3:00 PM – 5:00 PM

Exhibitors

101 375 South End Avenue Apt. 9G, New York, NY 10280, United States, Phone: 917-587-7883, Email: jb@101edu.co, Web: www.101edu.co, *101 develops Chem101, the next-generation active learning platform for chemistry courses.*
1107

AAAS/Science & Technology Policy Fellowship 1200 New York Ave., NW, Washington, DC 20005, United States, Phone: 202-326-6700, Fax: 202-289-4950, Email: fellowships@aaas.org, Web: go.stpf-aaas.org, *AAAS S&T Policy Fellowships provides opportunities to learn first-hand about federal policymaking while using your knowledge and analytical skills to address today's most pressing societal challenges.*
1122

abcr GmbH Im Schlehert 10 , Karlsruhe, 76187, Germany, Phone: +49 721 950 61101, Fax: +49 721 950 6133, Email: j.ehle@abcr.de, Web: www.abcr.de, *abcr. Gute Chemie - passion for the production, sale, research and development of special chemicals. Gute Chemie - created in Germany & Europe.*
915

Ace Glass, Inc. 1430 N. West Blvd. POBox 688, Vineland, NJ 08360, United States, Phone: 800-223-4524, Fax: 800-543-6752, Email: marketing@aceglass.com, Web: www.aceglass.com, *Ace Glass Inc has been a leader and innovator of scientific glassware and lab equipment for over 80 years, providing a wide variety of quality US manufactured standard and custom products.*
208

Acrotein ChemBio Inc. 2194 Suite K, Parkway Lake Drive, Hoover, AL 35244, United States, Phone: 205-730-9388, Fax: 205-730-9519, Email: sales@acrotein.com, Web: www.acrotein.com, *Acrotein ChemBio Inc. is a US-based supplier and manufacturer of special research chemicals: unnatural amino acids organic acids, amines, heterocycles & inhibitors etc. 8000+ rare compounds in stock.*
814

ACS Benefits, Programs, Services 1155 16th St. NW, Washington, DC 20036, United States, Phone: 202-872-4600, Email: c_allender@acs.org, Web: www.acs.org
637

ACS Career Fair 1155 16th Street, NW , Washington, DC 20036, United States *Get personalized career advice from an ACS Career Consultant, sign up for a mock-interview, upload your resume, and visit recruiters in the Exhibit Hall & Career Fair.*
1053

ACS Division of Small Chemical Businesses (SCHB) 4344 Moorpark Ave. Ste # 1, San Jose, CA 95129, United States, Phone: 408-834-8597, Fax: 408-351-7900, Email: expo-booth@acs-schb.org, Web: www.acs-schb.org, *SCHB is a network of entrepreneurs for formation- growth of small chemical businesses. It organizes programs on legal, educational, regulatory, economic aspects of business. Take part in lively Expo.*
1141

ACS Education 1155 16th Street, NW , Washington, DC 20036, United States, Phone: 202-872-6269, Fax: 202-833-7732, Email: education@acs.org, Web: www.acs.org/education, *ACS Education Division serves learners and educators by building communities and providing education resources, grants,professional development opportunities, and guidelines.*
637

ACS Green Chemistry Institute 1155 16th Street, NW , Washington, DC 20036, United States, Phone: 202-872-6102, Fax: 202-776-8009, Email: gci@acs.org, Web: www.acs.org/gci
646

ACS Meetings & Expositions 1155 Sixteenth Street NW , Washington, DC 20036, United States, Phone: 800-227-5558, Fax: 202-872-6128, Email: b_kashawlic@acs.org, Web: www.

acs.org/meetings

637

ACS Member Insurance Program 1155 16th Street, N.W. , Washington, DC 20036, United States, Phone: 800-227-5558-6037, Fax: 202-872-4435, Email: memins@acs.org, Web: www.acs.org/insurance, *Explore a wide array of insurance solutions available to ACS members, such as Life & Disability Insurance, Auto & Homeowners, Long Term Care, Professional Liability and more.*

637

ACS Membership 1155 16th St., NW Suite OTH420, Washington, DC 20036, United States, Phone: 202-872-6062, Email: j_gardiner@acs.org, Web: www.acs.org/memberhandbook

637

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637

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309

University Science Books 20 Edgehill Rd. , Mill Valley, CA 94941, United States, Phone: 415-332-5390, Fax: 415-383-3167, Email: univscibks@igc.org, Web: www.uscibooks.com, *Displaying fine new titles in chemistry, including Schrier's INTRODUCTION TO COMPUTATIONAL PHYSICAL CHEMISTRY, Wulfsberg's FOUNDATIONS OF INORGANIC CHEMISTRY, and Smith's THE BOLTZMANN FACTOR.*

428

Vacuubrand, Inc. 11 Bokum Rd. , Essex, CT 06426, United States, Phone: 860-767-2562, Fax: 860-767-2563, Email: kpouliot@brandtech.com, Web: www.vacuubrand.com

426

Vacuum Atmospheres Co. 4652 West Rosecrans Ave , Hawthorne, CA 90250, United States, Phone: 310-644-0255, Fax: 310-970-0980, Email: info@vac-atm.com, Web: www.vac-atm.com, *VAC has set the standards for gloveboxes and inert gas purification for over 50 years. Once again, our ongoing research and development has produced a proven revolutionary design. NO REGENERATION.*

218

Vacuum Technology Inc. 15 Great Republic Drive, Unit #4 , Gloucester, MA 01930, United States, Phone: 978-879-4302, Fax: 978-879-4387, Email: eva.zhang@vti-glovebox.com, Web: www.vti-glovebox.com, *Vacuum Technology Inc. builds and services the glove box needs of educational and industrial clients worldwide by integrating best-in-class components sourced from Europe, Asia, UK and the USA.*

445

Vapourtec Ltd. Unit 21, Park Farm Business Centre Fornham St Genevieve, Bury St Edmunds, Suffolk IP28 6TS, , United Kingdom, Phone: +44 (0) 1284 728659, Fax: +44 (0) 1284 728352, Email: duncan.guthrie@vapourtec.com, Web: www.vapourtec.com

536

Vernier Software & Technology 13979 SW Millikan Way, Beaverton, OR 97005, United States, Phone: 888-837-6437, Fax: 503-277-2440, Email: info@vernier.com, Web: www.vernier.com, *Educators worldwide use Vernier scientific data-collection technology, including a benchtop gas chromatograph and spectrophotometers, to teach and engage students in chemistry investigations.*

729

Vescent Photonics | New Exhibitor 6770 W. 52nd Ave., Suite B , Arvada, CO 80002, United States, Phone: 303-296-6766, Email: info@vescent.com, Web: www.vescent.com, *We supply a fine line of precision control electronics as well as DBR diode lasers and electro-optic modules for spectroscopic applications, including frequency references and servo controllers.*

1130

Vigor Tech USA, LLC 5100 Westheimer Road Suite 200, Houston, TX 77056, United States, Phone: 716-200-1200, Email: info@vigor-glovebox.com, Web: www.vigor-glovebox.com, *Vigor Tech USA, LLC is the world's most innovative glovebox and purification system supplier. Vigor's patented sealing technology and high capacity purifiers are unbeatable. Your research wants one!*

204

W.W. Norton 500 Fifth Ave. , New York, NY 10110, United States, Phone: 212-790-4357, Fax: 212-790-4261, Email: hventura@wwnorton.com, Web: www.wwnorton.com,

507

Waters Corp. 34 Maple Street , Milford, MA 01757, United States, Phone: 508-482-2000, Fax: 508-482-2674, Email: info@waters.com, Web: www.waters.com, *Waters Corp., the world's leading specialty measurement company, has pioneered chromatography, mass spec and thermal analysis innovations serving the life, materials and food sciences for 60 years.*

703

Wavefunction, Inc. 18401 Von Karman Suite 370, Irvine, CA 92612, United States, Phone: 949-955-2120, Fax: 949-955-2118, Email: sales@wavefun.com, Web: www.wavefun.com, *Wavefunction, Inc. provides Spartan and Odyssey molecular modeling solutions. Cutting edge software for research and education. Now available...Spartan'18 Parallel Suite.*

501

Welch by Gardner Denver 1601 Feehanville Drive Suite 550, Mount Prospect, IL 60056, United States, Phone: 847-676-8800, Fax: 847-677-8606, Email: mark.suda@gardnerdenver.com, Web: www.welchvacuum.com, *Welch is the global leader in applied vacuum technology. Welch is featuring the new CRVpro rotary vane vacuum pump family, flow rates up to 22 cfm, with advanced features to extend service intervals.*

441

Wiley | Sponsor 111 River St. , Hoboken, NJ 07030, United States, Phone: 201-748-6000, Email: clkelly@wiley.com, Web: www.wiley.com, *Wiley's product diversity is unique, spanning books, journals, databases, web-portals & workflow tools. Visit Booth #409 to see what's new. All onsite books orders are 30% off with free shipping!*

409

Wilmad-LabGlass 1172 N.W. Boulevard , Vineland, NJ

08360, United States, Phone: 856-691-3200, Fax: 856-691-6206, Email: cs@wilmad-labglass.com, Web: www.wilmad-labglass.com, *Wilmad-LabGlass provides over 7,000 products including NMR / EPR consumables and specialty glassware, as well as custom fabrication for individual glassware, glass repair services and OEM glass parts.*
527

Workrite Uniform Company 1701 North Lombard St. , Oxnard, CA 93030, United States, Phone: 800-521-1888, Fax: 805-483-0678, Email: info@workrite.com, Web: www.workritefrcp.com, *Workrite Uniform Company has a new lab coat and coverall that provides flame-resistant properties and chemical splash protection. It's the first of it's kind in offering simultaneous protection.*
826

Wyatt Technology Corp. 6300 Hollister Avenue , Santa Barbara, CA 93117, United States, Phone: 805-681-9009, Fax: 805-681-0123, Email: info@wyatt.com, Web: www.wyatt.com, *Wyatt Technology provides instruments for determining the absolute molar mass, size, charge and interactions of macromolecules and nanoparticles in solution with multi-angle light scattering (MALS).*
619

X-Ability Co., Ltd. Ishiwata Building, 3rd Floor 4-1-5 Hongo, Bunkyo-Ku, Tokyo, 113-0033, Japan, Phone: +81-3-5800-7731, Email: rkoga@x-ability.jp, Web: www.x-ability.co.jp
1133

ACS Career Fair

Job seekers, are you looking to jump-start job search or enhance your professional development?

Employers, are you looking to hire scientists and engineers?

Then you need to attend the ACS Career Fair, open Sunday-Tuesday, March 18-20, 9:00 AM to 5:00 PM. The career fair is the place where the best talent and the best employers in chemistry meet.

The ACS Career Fair provides on-site activities for job seekers to help them reach their career goals. ACS will help you prepare for your next career move by providing resources that make it possible to map out your personal job search strategy, strengthen your resume, and build your interview skills, all with the support of career consultants.

During the career fair, ACS members can take full advantage of the following:

- Networking opportunities
- Resume reviews
- One-on-one career consulting
- Interview practice and skills building
- Career-related workshops
- Keynote speakers presented live and via webcast
- Live, on-site interviews on request

Not an ACS member? You are welcome to network and engage with employers on the expo floor.

Please note: We cannot guarantee that you will secure interviews at the ACS Career Fair. Interviewing is strictly contingent on the availability of positions and the credentials and qualifications that employers are seeking.

One-On-One Career Consulting

Individual, 30-minute appointments with career consultants are available on-site and online. These consultants can help you strengthen your resume, improve your interviewing skills, and design a job search or comprehensive professional growth strategy. Please bring a copy of your resume or CV to all appointments. All one-on-one on-site career consulting sessions will take place in the Resume Review/Mock Interview area in the ACS Career Fair. Sign-up begins 9:00 am on Sunday, March 18, on a first-come, first-served basis.

GOVERNANCE & BUSINESS MEETINGS

Many members participate in meetings concerning the business of the Society, technical divisions, and governance committees in conjunction with the National Meeting. The following pages list the open meetings scheduled for New Orleans, LA. ACS encourages its members to get active in governance at all levels in order to contribute their vision to the direction of the Society.

You can share ideas and insights into the Society and the chemical profession, network with peers, and catch up friends through these volunteer connections. With nearly 30 national governance committees and leadership opportunities in technical divisions and local sections to choose from, there are many opportunities for members to become actively involved in ACS at the national level.

If you are an ACS member interested in volunteering for a governance committee, contact the Office of the Secretary at secretary@acs.org or by telephone at 202-872-4461. Someone will put you in contact with the ACS Committee on Committees to discuss your desire to volunteer for a committee assignment. If you wish to volunteer for a specific technical division or local section, contact the officers listed at www.acs.org to explore your specific interests.

ACS Board of Directors

The ACS Board of Directors meeting, open to all members who wish to participate, will be held at the Ernest N. Morial Convention Center from 12:00 PM to 1:00 PM on Sunday, March 18.

ACS Council

The ACS Council meeting will begin at 8:00 am, Wednesday, March 21, at the Hilton New Orleans Riverside Hotel. Councilor check in and a continental breakfast start at 7:00 am and will continue until the meeting opens at 8:00 am. Space will be available for ACS members and nonmembers to observe the council in action.

We hope that many will take advantage of this opportunity to learn firsthand about the Society's operation. Alternate councilors and division and local section officers are particularly urged to attend.

Council Policy Committee

The Council Policy Committee will open the floor during its meeting at 11:30 am on Tuesday, March 20, to councilors who would like to raise issues of concern that affect them and/or their local sections or divisions. For additional information, contact CPC Vice Chair Mary Carol at cpc@acs.org.

Committee on Committees Agenda

The Committee on Committees has clarified three types of committee meetings:

1. Closed

The committee chair must declare any executive session closed when confidential or sensitive personnel, financial, or legal matters of the Society are discussed. At that point, only officially appointed or elected committee members, associates, consultants, staff liaisons, and the appointed Committee on Committees liaison shall remain in the session. Others may stay in the session at the discretion of the chair. Once these discussions have been completed, the committee should return to executive mode.

2. Executive

Attendance and participation are limited to officially appointed or elected committee members, associates, advisers, consultants, staff liaisons, and the appointed Committee on Committees liaison. Committee chairs may extend meeting participation to other Committee on Committees liaisons, ex-officio officers, and elected councilors. Only committee members can vote.

3. Open

May be attended by any ACS member. At these sessions, members are encouraged to voice concerns, issue compliments, offer suggestions, and express interest in or raise questions about matters over which the committee has purview. The assumption is that participation is welcomed and will be orderly and courteous. Only committee members can vote.

During the Executive and Open committee meetings, ACS members will have an opportunity to express their views on issues under consideration before they are acted on by the board or the council. Members can also bring up other subjects that deserve attention. Members are urged to examine the agenda and make known any opinions or ideas they may have. If you are unable

to attend the meeting, send an email to the officer listed, or ask someone attending the session to speak on your behalf.

Governance and Business Meetings

All governance and business meetings will be held at the Hilton New Orleans Riverside unless noted otherwise.

Budget & Finance

Joseph A. Heppert, Chair, b_ffeedback@acs.org
Open Session: Saturday, March 17, 8:00 AM to 10:30 PM, Grand Ballroom B

Chemical Safety

Ralph Stuart, Chair, safety@acs.org
Open Executive Session: Saturday, March 17, 8:15 AM to 9:45 PM, Grand Ballroom B, and Monday, March 19, 7:00 AM to 8:30 AM

Chemistry & Public Affairs

Raymond E. Forslund, Chair, reforslund@me.com
Open Session: Saturday, March 17, 3:00 PM to 4:30 PM , Grand Ballroom C

Chemists with Disabilities

James Schiller, Chair, james.schiller@merck.com
Combined Open and Executive Session: Sunday, March 18, 8:30 AM to 4:30 PM, Grand Salon A Section 3/6

Committees

Carolyn Ribes, Chair, cribes@dow.com
Open Session: Monday, March 19, 1:30 PM to 2:00 PM , Grand Salon A Section 3/6

Community Activities

Michael B. McGinnis, Chair, outreach@acs.org
Closed Executive Session: Sunday, March 18, 7:00 AM to 12:00 PM, Grand Salon A Section 3/6

CCA/LSAC

Joint Open Session: Tuesday, March 20, 2:00 PM to 3:30 PM, Grand Salon A Section 3/6

Constitution & Bylaws

V. Dean Adams, Chair, bylaws@acs.org
Executive Session: Sunday, March 18, 10:00 AM to 11:30 AM and 1:45 PM to 4:30 PM
Open Session: Sunday, March 18, 1:30 PM to 1:45 PM, Grand Salon A Section 3/6

Corporation Associates

Diane Grob Schmidt, Chair, d_schmidt@acs.org
Open Session: Monday, March 19, 8:00 AM to 12:00 PM

Council Policy

Mary K. Carroll, Vice Chair, cpc@acs.org
Open Executive Session: Tuesday, March 20, 9:30 AM to 12:00 PM, St. Charles Ballroom

Divisional Activities

Rodney M. Bennett, Chair, rodbennettdac@gmail.com
Open Executive Session: Sunday, March 18, 8:00 AM to 12:00 PM, Kabacoff

Economic & Professional Affairs

Tiffany Hoerter, Chair, thoerter@gmail.com
Executive Session: Saturday, March 17, 8:00 AM to 3:00 PM
Open Session: Saturday, March 17, 3:00 PM to 5:30 PM, Grand Salon C Section 15/18

Education

Jennifer Nielson, Chair, jnielson@chem.byu.edu
Open Session Monday, March 19, 3:00 PM to 4:00 PM, Grand Salon B Section 12
Executive Session: Friday, March 16, 1:00 PM to 5:30 PM, Grand Salon C Section 15/18

Environmental Improvement

Anthony (Tony) Noce, Chair, cei@acs.org
Breakfast/Open Session: Monday, March 19, 7:45 AM to 9:00 AM, Ernest N. Morial Convention Center, Room 345

Ethics

Judith Currano, Chair, currano@pobox.upenn.edu
Open Executive Session: Sunday, March 18, 9:00 AM to 4:30 PM, Grand Salon B Section 10

International Activities

Jens Breffke, Chair, breffke@gmail.com
Open Session: Saturday, March 17, 1:00 PM to 3:00 PM, Chart A/B

Local Section Activities

Jason Ritchie, Chair, jritchie@olemiss.edu
LSAC/CCA Joint Open Session: Tuesday, March 20, 2:00 PM to 3:30 PM, Grand Salon B Section 9/12
Open Executive Session: Sunday, March 18, 8:00 AM to 12:00 PM, Grand Ballroom D

Meetings & Expositions

Kevin J. Edgar, Chair, M&E@acs.org
Closed Executive Session Sunday, March 18, 10:00 AM to 12:00 PM, Ernest N. Morial Convention Center, Room 206
Open Session: Sunday, March 18, 7:30 AM to 10:00 AM, Ernest N. Morial Convention Center, Room 206

Membership Affairs

Margaret J. Schooler, margaret.j.schooler@axaltacs.com
Closed Executive Session: Sunday, March 18, 7:15 AM to 3:00 PM, Jefferson Ballroom
Open Executive Session Sunday, March 18, 3:00 PM to 4:00 PM, Jefferson Ballroom

Minority Affairs

Ann Kimble-Hill, Chair, ankimble@umail.iu.edu
Closed Executive Session: Sunday, March 18, 8:00 AM to 12:30 PM, Grand Ballroom C
Open Session: Sunday, March 18, 12:30 PM to 2:00 PM, Grand Ballroom C

Nomenclature, Terminology & Symbols

Michael D. Mosher, Chair, michael.mosher@unco.edu
Open Session: Monday, March 19, 2:00 PM to 5:00 PM, Grand Ballroom B

Nominations & Elections

Les W. McQuire, Chair, nomelect@acs.org
Open Executive Session: Monday, March 19, 11:30 AM to 12:00 PM, Marlborough B

Patents & Related Matters

Kirby Drake, Chair, kirby.drake@klemchuk.com
Open Session: Saturday, March 17, 9:00 AM to 4:00 PM, Windsor

Professional Training

Edgar Arriaga, Chair, cpt@acs.org
Open Session: Sunday, March 18, 4:00 PM to 6:00 PM, Renaissance New Orleans Arts Hotel, Patrons Ballroom III

Project SEED

Don Warner, Chair, dwarner@boisestate.edu
Closed Executive Session: Saturday, March 17, 10:30 AM to 5:00 PM, Grand Salon B Section 9
Open Session: Sunday, March 18, 9:30 AM to 10:30 AM, Burgundy

Public Relations & Communications

Jennifer Maclachlan, Chair, pidgirl@gmail.com
Open Executive Session: Monday, March 19, 8:00 AM to 1:00 PM, Kabacoff

Publications

Nicole S. Sampson, Chair, nicole.sampson@stonybrook.edu
Closed Executive Session: Friday, March 16, 1:00 PM to 5:00 PM, Ascot/Newberry
Open Session: Friday, March 16, 4:30 PM to 5:00 PM, Ascot/Newberry

Science

Mark C. Cesa, Chair, markcesa@comcast.net
Open Session: Saturday, March 17, 8:30 AM to 4:30 PM, Grand Salon A Section 3/6

Senior Chemists

Thomas R. Beattie, Chair, seniorchemists@acs.org
Open Executive Session: Monday, March 19, 8:00 PM to 1:00 PM, Compass

Technician Affairs

Aimee Tomlinson, Chair, cta@acs.org
Closed Executive Session: Sunday, March 18, 8:00 AM to 12:30 PM
Open Executive Session: Sunday, March 18, 12:30 PM to 1:00 PM, St. James Ballroom

Women Chemists

Kimberly A. Woznack, Chair, wcc@acs.org
Executive Session: Saturday, March 17, 8:00 AM to 5:00 PM, Jefferson Ballroom

Younger Chemists

Natalie A. LaFranzo, Chair, nlafranzo@gmail.com
Closed Session: Saturday, March 17, 8:00 AM to 3:00 PM, St. James Ballroom
Open Session: Sunday, March 18, 8:00 AM to 12:00 PM, Chart C

For the complete list of committee meetings with the associated agenda, please visit the meeting website, **www.acs.org/nationalmeeting.**

Councilor Caucus Meetings

All Councilor Caucus Meetings will be held on Sunday, March 18, from 6:00 PM to 7:00 PM at the Hilton New Orleans Riverside unless noted otherwise.

District I Councilor Caucus,Chart A
District II Councilor Caucus, Chart B
District III Councilor Caucus, Chart C
District IV Councilor Caucus, Kabacoff
District V Councilor Caucus, Port
District VI Councilor Caucus, Starboard
Division Officers/Councilors Caucus, Grand Salon B Section 7
Tuesday, March 20, 4:00 PM to 6:00 pm

DIVISION MEETINGS AND SOCIAL EVENTS

Division of Analytical Chemistry – ANYL

ANYL Poster Session	Sunday, March 18	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall E

Division of Agriculture & Food Chemistry – AGFD

AGFD Special Topics Meeting	Sunday, March 18	12:00 PM – 1:00 PM	Ernest N. Morial Convention Center	Room 218
AGFD Poster Session and Reception	Sunday, March 18	5:30 PM – 8:00 PM	Ernest N. Morial Convention Center	Hall E
General & AGFD All-Star Posters	Sunday, March 18	5:30 PM – 7:30 PM	Ernest N. Morial Convention Center	Hall E
AGFD Future Programs Meeting	Sunday, March 18	12:00 PM – 1:00 PM	Ernest N. Morial Convention Center	Room 218
AGFD Executive Committee Meeting	Monday, March 19	5:30 PM – 8:30 PM	Ernest N. Morial Convention Center	Room 218
C4, Communicating Chemistry: Â Creole Cooking	Tuesday, March 20	10:30 PM – 1:30 PM	Off-Site	Dickie Brennan's Steakhouse 716 Iberville Street

Division of Biological Chemistry – BIOL

BIOL Current Topics Posters	Sunday, March 18	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall E
ACS Chemical Biology Lectureship Award Reception	Tuesday, March 20	12:00 PM – 1:30 PM	Ernest N. Morial Convention Center	Room 244
BIOL Current Topics Posters	Tuesday, March 20	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall E

Division of Biochemical Technology – BIOT

BIOT Strategic Planning Meeting	Saturday, March 17	8:00 AM – 4:00 PM	InterContinental New Orleans	Poydras Room
BIOT Future Programming Meeting	Tuesday, March 20	12:30 PM – 2:00 PM	InterContinental New Orleans	La Salle B/C
BIOT Poster Session	Tuesday, March 20	6:00 PM – 8:00 PM	Ernest N. Morial Convention Center	Hall E

Division of Carbohydrate Chemistry – CARB

ACS Division of Carbohydrate Chemistry - Strategic Planning Meeting	Saturday, March 17	3:00 PM – 9:00 PM	Loews New Orleans Hotel	St. Landry
NIH - Facile Methods and Technologies for Synthesis of Biomedically Relevant Carbohydrates (U01)	Sunday, March 18	5:00 PM – 7:00 PM	Le Meridien New Orleans	Salon 7
ACS Division of Carbohydrate Chemistry - Executive Committee Meeting	Monday, March 19	7:00 PM – 10:00 PM	Le Meridien New Orleans	Salon 6
CARB Awards Dinner	Monday, March 19	7:00 PM – 10:00 PM	Off-Site	Hilton New Orleans/St. Charles Avenue, 333 St. Charles Avenue
CARB General Posters	Monday, March 19	7:30 PM – 9:30 PM	Ernest N. Morial Convention Center	Hall E

Division of Cellulose and Renewable Materials - CELL

CELL Executive Committee Meeting	Saturday, March 17	4:00 PM – 7:30 PM	Loews New Orleans Hotel	Point Coupee
CELL Poster Session	Sunday, March 18	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall D
CELL Awards Banquet	Tuesday, March 20	6:00 PM – 10:00 PM	Pat O'Brien's on the River	600 Decatur Street
CELL Business Meeting	Wednesday, March 21	5:30 PM – 7:00 PM	Loews New Orleans Hotel	Lafourche
CELL Technical Programming Meeting	Wednesday, March 21	7:00 PM – 8:00 PM	Loews New Orleans Hotel	Lafourche

Division of Chemical Education – CHED

DivCHED Finance Committee Meeting	Friday, March 16	3:00 PM – 6:30 PM	New Orleans Marriott Convention Center	Fleur De Lis
ACS Exams Institute Board of Trustees Meeting	Saturday, March 17	7:30 PM – 12:00 PM	New Orleans Marriott Convention Center	Blaine Kern A
Journal of Chemical Education Board of Publication Meeting	Saturday, March 17	7:30 PM – 12:00 PM	New Orleans Marriott Convention Center	Blaine Kern B
ACS Exams Committee 1	Saturday, March 17	8:00 AM – 5:00 PM	Le Meridien New Orleans	Uptown 1-3
ACS Exams Committee 2	Saturday, March 17	8:00 AM – 5:00 PM	Le Meridien New Orleans	Salon 3
ACS Exams Committee 3	Saturday, March 17	8:00 AM – 5:00 PM	Le Meridien New Orleans	Salon 6
ACS Exams Committee 4	Saturday, March 17	8:00 AM – 5:00 PM	Le Meridien New Orleans	Salon 7
DivCHED Biennial Conference Committee Meeting	Saturday, March 17	10:30 AM – 12:00 PM	New Orleans Marriott Convention Center	Julia
DivCHED Program Committee Meeting	Saturday, March 17	10:30 AM – 12:00 PM	New Orleans Marriott Convention Center	River Bend 1/2
DivCHED Executive Committee Meeting	Saturday, March 17	10:30 AM – 12:00 PM	New Orleans Marriott Convention Center	River Bend 1/2
DivCHED Pre-college Committee	Saturday, March 17	5:00 PM – 8:00 PM	Ernest N. Morial Convention Center	Room 215
ACS Exams Workshop	Sunday, March 18	8:00 AM – 5:00 PM	Le Meridien New Orleans	Salon 1/2
DivCHED International Activities Committee Meeting	Sunday, March 18	8:00 AM – 10:00 PM	Hilton Garden Inn Convention Center	Carmellia Room
ACS DivCHED Regional Meetings Committee Meeting	Sunday, March 18	12:00 PM – 2:00 PM	Hilton Garden Inn Convention Center	St. Charles Room
Chemistry Educators Luncheon	Sunday, March 18	12:00 PM – 1:00 PM	New Orleans Marriott Convention Center	Blaine Kern C/D
DivCHED Chemical Education Research Committee Meeting	Sunday, March 18	12:00 PM – 1:30 PM	Hilton Garden Inn Convention Center	Carmellia Room

Division of Chemical Education – CHED (contd.)

DivCHED Long Range Planning Committee Meeting	Sunday, March 18	2:30 PM – 4:30 PM	Hilton Garden Inn Convention Center	Carmellia Room
DivCHED Safety Committee Meeting	Sunday, March 18	4:00 PM – 5:30 PM	Hilton Garden Inn Convention Center	St. Charles Room
DivCHED Business Meeting	Sunday, March 18	4:30 PM – 5:00 PM	Hilton Garden Inn Convention Center	Carmellia Room
Division of Chemical Education Social Reception	Sunday, March 18	5:30 PM – 7:00 PM	Ernest N. Morial Convention Center	Great Hall D
General Posters	Sunday, March 18	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall D
ACS Exams Workshop	Monday, March 19	8:00 AM – 5:00 PM	Le Meridien New Orleans	Salon 1/2
DivCHED Younger Chemistry Education Scholars Committee Meeting	Monday, March 19	12:00 PM – 2:00 PM	Hilton Garden Inn Convention Center	Gardenia Room
Undergraduate Research Posters	Monday, March 19	12:00 PM – 2:00 PM	Ernest N. Morial Convention Center	Halls D/E
DivCHED New Member Meeting	Monday, March 19	12:30 PM – 2:30 PM	Hilton Garden Inn Convention Center	Carmellia Room
Graduate Student Symposium Information Session	Monday, March 19	1:00 PM – 1:30 PM	Hilton Garden Inn Convention Center	Carmellia Room
Two-Year College Chemistry Consortium Meeting	Monday, March 19	3:00 PM – 5:00 PM	Hilton Garden Inn Convention Center	Carmellia Room
Successful Student Chapters	Monday, March 19	8:00 PM – 10:00 PM	Ernest N. Morial Convention Center	Halls D/E

Division of Colloid and Surface Chemistry - COLL

COLL Program & Executive Committee Meeting	Saturday, March 17	4:00 PM – 7:00 PM	Ernest N. Morial Convention Center	Room 237
COLL Poster Session	Sunday, March 18	6:00 PM – 8:00 PM	Ernest N. Morial Convention Center	Halls B2/C

Division of Computers in Chemistry - COMP

Computers in Chemistry Programming and Executive Committee Meeting	Saturday, March 17	3:00 PM – 6:00 PM	New Orleans Marriott Convention Center	Blaire Kern B
COMP Poster Session	Tuesday, March 20	Tuesday, March 20	Ernest N. Morial Convention Center	Hall E

Division of Geochemistry – GEOC

GEOC Executive Committee Meeting	Sunday, March 18	6:00 PM – 8:00 PM	Ernest N. Morial Convention Center	Room 213
GEOC Poster Session	Wednesday, March 21	6:00 PM – 8:00 PM	Ernest N. Morial Convention Center	Hall D

Division of Inorganic Chemistry – INOR

INOR Poster Session	Sunday, March 18	5:30 PM – 7:30 PM	Ernest N. Morial Convention Center	Hall D
INOR Poster Session	Tuesday, March 20	5:30 PM – 7:30 PM	Ernest N. Morial Convention Center	Hall D

Division of Industrial and Engineering Chemistry – I&EC

I&EC Division Committee Meetings	Saturday, March 17	12:00 PM – 4:00 PM	Loews New Orleans Hotel	Lafourche
I&EC Division Open Meeting	Saturday, March 17	4:00 PM – 5:00 PM	Loews New Orleans Hotel	Lafourche

Division of Medicinal Chemistry – MEDI

Strategic Meeting	Saturday, March 17	8:30 AM – 5:30 PM	Ernest N. Morial Convention Center	Room 210
MEDI Business Meeting	Sunday, March 18	5:30 PM – 6:30 PM	Ernest N. Morial Convention Center	Room 216
MEDI Executive Committee	Sunday, March 18	8:30 AM – 1:00 PM	Hilton Garden Inn Convention Center	Gardenia Room
MEDI Long Range Planning Committee Meeting	Monday, March 19	5:30 PM – 10:30 PM	Ernest N. Morial Convention Center	Room 215
MEDI General Posters	Sunday, March 18	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall E
MEDI/ORGN Poster Session	Wednesday, March 21	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall B1

Division of Organic Chemistry - ORGN

ORGN Poster Session	Sunday, March 18	5:30 PM – 7:30 PM	Ernest N. Morial Convention Center	Hall D
ORGN Poster Session	Tuesday, March 20	5:30 PM – 7:30 PM	Ernest N. Morial Convention Center	Hall D
MEDI/ORGN Poster Session	Wednesday, March 21	7:00 PM – 9:00 PM	Ernest N. Morial Convention Center	Hall B1
ORGN Executive Committee Meeting	Sunday, March 18	1:00 PM – 6:00 PM	Ernest N. Morial Convention Center	Room 206

Division of Polymeric Materials: Science and Engineering - PMSE

PMSE Membership Desk	Saturday, March 17	8:00 AM – 5:00 PM	New Orleans Marriott Canal Street	Studio Foyer
PMSE Membership Desk	Sunday, March 18	8:00 AM – 5:00 PM	New Orleans Marriott Canal Street	Studio Foyer
PMSE Executive Committee	Sunday, March 18	4:30 PM – 7:30 PM	Astor Crowne Plaza New Orleans	St. Charles Ballroom A/B
PMSE Membership Desk	Monday, March 19	8:00 AM – 5:00 PM	New Orleans Marriott Canal Street	Studio Foyer
PMSE Business Meeting & PMSE/POLY Coordination Meeting	Monday, March 19	5:00 PM – 6:00 PM	New Orleans Marriott Canal Street	Studio 9
PMSE Membership Desk	Tuesday, March 20	8:00 AM – 5:00 PM	New Orleans Marriott Canal Street	Studio Foyer
Joint PMSE/POLY Poster Session	Tuesday, March 20	6:00 AM – 8:00 PM	Ernest N. Morial Convention Center	Hall E
PMSE Membership Desk	Wednesday, March 21	8:00 AM – 5:00 PM	New Orleans Marriott Canal Street	Studio Foyer
POLY/PMSE Plenary Award Session	Wednesday, March 21	5:30 AM – 8:00 PM	New Orleans Marriott Canal Street	Acadia
PMSE Membership Desk	Thursday, March 22	8:00 AM – 12:00 PM	New Orleans Marriott Canal Street	Studio Foyer

Division of Polymer Chemistry - POLY

PMSE Membership Desk	Sunday, March 18	12:00 PM – 2:00 PM	Astor Crowne Plaza New Orleans	St. Charles Ballroom A/B
PMSE Membership Desk	Sunday, March 18	2:00 PM – 3:00 PM	Astor Crowne Plaza New Orleans	Burgundy
PMSE Executive Committee	Sunday, March 18	3:00 PM – 4:00 PM	Astor Crowne Plaza New Orleans	Burgundy
PMSE Membership Desk	Sunday, March 18	4:00 PM – 5:30 PM	Astor Crowne Plaza New Orleans	Burgundy
PMSE Business Meeting & PMSE/POLY Coordination Meeting	Monday, March 19	12:30 PM – 2:00 PM	Astor Crowne Plaza New Orleans	Burgundy
PMSE Membership Desk	Tuesday, March 20	9:00 AM – 12:00 PM	Astor Crowne Plaza New Orleans	Burgundy
Joint PMSE/POLY Poster Session	Tuesday, March 20	1:00 PM – 2:00 PM	Astor Crowne Plaza New Orleans	St. Charles Ballroom A/B

Division of Polymer Chemistry - POLY (contd.)

PMSE Membership Desk	Tuesday, March 20	2:00 AM – 3:00 PM	Astor Crowne Plaza New Orleans	Burgundy
POLY/PMSE Plenary Award Session	Tuesday, March 20	6:00 PM – 8:00 PM	Ernest N. Morial Convention Center	Hall E

Division of Small Chemical Businesses – SCHB

SCHB Business Meetings	Saturday, March 17	7:00 PM – 7:15 PM	Loews New Orleans Hotel	Lafourche
SCHB Executive Committee	Saturday, March 17	7:15 PM – 9:00 PM	Loews New Orleans Hotel	Lafourche
SCHB Poster Session	Sunday, March 18	6:00 PM – 8:00 PM	Ernest N. Morial Convention Center	Halls B2/C

STUDENT AND EDUCATOR ACTIVITIES

Undergraduate students, graduate students, high school teachers, and chemical professionals will have the opportunity to participate in a number of education-focused programs and specialty activities.

Chemistry Teachers Day Program

The Division of Chemical Education and the ACS Education Division are sponsoring the Chemistry Teacher Program. It will include presentations on current pedagogies, resources, and activities.

The High School-College Interface Luncheon will bring together educators from all grade levels with the goal of facilitating an exchange of ideas and networking among teachers and professors.

Sunday, March 18, 8:00 am to 5:00 pm, New Orleans Marriott Convention, Blaine Kern C/D.

Participation requires a separate registration. If you need to register, you can do so in the Attendee Registration Office, Lounge A in the Convention Center Rivergate Ballroom.

Workshops

Laboratory Waste Management

Presenter: Russ Phifer

CHAS offers the Laboratory Waste Management workshop to assist participants with the various regulatory requirements that apply to laboratories, which generate hazardous waste, as well as to provide insight into the options for on-site management and off-site disposal. Focus will include discussion on recycling/reclamation techniques, economical handling of wastes and liability issues. There is extensive opportunity for questions both during the workshop with follow-up by phone and email.

Laboratory Safety Workshop – Beyond the Fundamentals

Presenter: Jim Kaufman

The Laboratory Safety Workshop– Beyond the Fundamentals is a new ACS National Meetings course offered by the Laboratory Safety Institute, The goal of the course is to meet the needs of scientists and science educators wanting to learn more about laboratory safety. "Lab Safety–Beyond the Fundamentals" continues where LSI's introductory course (The Laboratory Safety Workshop) leaves off and explores new areas in lab safety. There is an emphasis on simple and inexpensive steps to create more effective lab safety programs and grow the culture of lab safety. There is extensive opportunity for questions both during the workshop with follow-up by phone and email. This includes a one-hour conference call to help with the implementation of course concepts.

Course participants are encouraged to submit in advance five questions/topics they wish to have addressed in the course. Send questions/topics to: jim@labsafetyinstitute.org

How to Be a More Effective Chemical Hygiene Officer

Presenter: Russ Phifer

CHAS offers the How to be a more effective Chemical Hygiene Officer workshop to provide participants with a detailed analysis of the CHO position and to prepare for the "CHO" Certification exam. Participants receive a clear perspective on safety issues in the laboratory, focusing on what the CHO does and how to do it better. The workshop covers the content areas of the certification exam, including a sample test in the same format as the real one. Whether you are a new Chemical Hygiene Officer or an "old" one, you will find something to put to real use in this fast-paced presentation.

There is extensive opportunity for questions during the workshop and with follow-up by phone and email.

Reactive Chemical Management for Laboratories & Pilot Plants

Presenters: Neal Langerman, Harry Elston

Chemical reactivity hazards contribute to a significant number of incidents in laboratories and pilot plants. This workshop will provide participants with the knowledge and skill to screen processes for potential hazards, recognize when reactive hazards are present, and implement appropriate controls to reduce the risk of an incident associated with the hazards. Workshop attendees will review case studies of actual incidents and do screening examples in order to understand the screening and recognition process. Group discussions of control methods will allow participants to share their experiences and to evaluate methods for controlling reactivity risks.

Developing Graduate Student Leadership Skills in Laboratory Safety

Presenters: Kali Serrano of the University of Illinois and Michail Vlysidis of University of Minnesota

Co-sponsor: ACS Committee on Chemical Safety and the ACS Office of Graduate Education

Recently, several research-intensive chemistry departments have instituted Joint Safety Teams (JSTs) and similar programs to support graduate student empowerment around laboratory safety issues. This three-hour workshop will describe these efforts at the University of Illinois and University of Minnesota as well as literature from the ACS and the National Academy of Sciences that describes the opportunities and challenges of safety culture in the academic environment. These topics will be followed by discussion of practical steps graduate students can take at their institution to support improved safety cultures. The presenters are graduate students with hands-on experience in the workshop focus. Leadership of the ACS Division of Chemical Health and Safety will provide technical support. Participants will receive a "Graduate Student Safety Leader" certificate.

ACS Career Navigator

ACS Career Navigator is your home for career services, leadership development, professional education, and market intelligence resources. We offer comprehensive and easily identified tools to help you achieve your career goals by landing a new job, finding a new career path, comparing your salary, and viewing current trends in the chemistry enterprise to make more informed decisions.

Opportunities for career development abound at the ACS National Meeting in New Orleans. Take advantage of the resources and tools the ACS Career Navigator offers to help you succeed in the global scientific enterprise. Are you ready to get started? Refresh your skills and branch into new areas of emerging science and advanced applications with an ACS Short Course. Take an ACS Leadership Development System course to gain skills that can be immediately applied in school or on the job. If you are an ACS member, stop by the ACS Career Fair in the Ernest N. Morial Convention Center to speak to a personal career consultant or to have a professional head shot taken. In short, whatever your career goals, the ACS Career Navigator is here to help you achieve and exceed them.

Career and Professional Development Workshops

Our career-related workshops on varying topics will help you with everything from improving your resume to optimizing job performance to acing an interview. Workshop times are subject to change. Please consult the online workshop schedule at the meeting website.

Sunday, March 18

- New Technology to Find Jobs & Manage Your Career, 9:00 AM - 10:30 AM
- ChemIDP- Planning for Your Career, 11:00 AM - 12:45 PM
- Finding Yourself: Identifying a Career that Matches your Strengths and Values, 1:00 PM - 4:00 PM
- Networking: How to Get Started, 4:30 PM - 5:30 PM
- Setting Yourself Up for Success in an Interview, 1:00 PM - 3:00 PM
- Making the Most of Your Interview: Outshine the Competition, 3:30 PM - 5:30 PM
- Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 1:00 PM - 3:00 PM
- Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 3:30 PM - 5:30 PM

Monday, March 19

- Opportunities for Chemists in the Federal Government, 8:00 AM - 10:00 AM
- Finding Your Market, Defining Your Business, 8:00 AM - 10:00 AM
- How to Find and Apply for a Chemistry Position in the Federal Government, 10:30 AM - 12:30 PM
- Your Sales Marketing and Financing Plan, 10:30 AM - 12:30 PM
- Finding Yourself: Identifying a Career that Matches your Strengths and Values, 1:00 PM - 4:00 PM
- Networking: How to Get Started, 4:30 PM - 5:30 PM
- Setting Yourself Up for Success in an Interview, 1:00 PM - 3:00 PM
- Making the Most of Your Interview: Outshine the Competition, 3:30 PM - 5:30 PM
- The Higher Ed Landscape, 8:00 AM - 10:00 AM
- Higher Ed-Presenting Yourself, 10:30 AM - 12:30 PM
- Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 1:00 PM - 3:30 PM
- Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 3:30 PM - 5:30 PM

Tuesday, March 20

- Finding Yourself: Identifying a Career that Matches your Strengths and Values, 8:00 AM - 11:00 AM
- Networking: How to Get Started, 11:30 AM - 12:30 PM
- Opportunities for Chemists in the Federal Government, 1:00 PM - 3:00 PM
- How to Find and Apply for a Chemistry Position in the Federal Government, 3:30 PM - 5:30 PM
- Setting Yourself Up for Success in an Interview, 8:00 AM - 10:00 AM
- Making the Most of Your Interview: Outshine the Competition, 10:30 AM - 12:30 PM
- Foreign National Scientist Obtaining a Job in the U.S, 1:30 PM - 3:00 PM
- Writing Excellent Proposals, 3:30 PM - 5:00 PM
- Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 8:00 AM - 10:00 AM
- Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 10:30 AM - 12:30 PM
- The Higher Ed Landscape, 1:00 PM - 3:00 PM
- Higher Ed-Presenting Yourself, 3:30 PM - 5:30 PM

Wednesday, March 21

- Finding Yourself: Identifying a Career that Matches your Strengths and Values, 8:00 AM - 11:00 AM
- Networking: How to Get Started, 11:30 AM - 12:30 PM
- Setting Yourself Up for Success in an Interview, 8:00 AM - 10:00 AM
- Making the Most of Your Interview: Outshine the Competition, 10:30 AM - 12:30 PM
- Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 8:00 AM - 10:00 AM
- Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 10:30 AM - 12:30 PM

ACS Professional Education Short Courses

The following short courses, specifically designed to improve the skills and marketability of chemical scientists and technicians, are offered in conjunction with the national meeting. ACS member, early registration, and group discount rates are available. Register for these courses when you register for the meeting. For more information on ACS Short Courses, to obtain pricing details, or to view a full course catalog, visit www.proed.acs.org/neworleans2018. If you have questions, call (202) 872-4508, fax (202) 872-6336, or email proed@acs.org.

Computers/Statistics/Engineering

- Chemical Engineering for Chemists, March 17-18
- Experimental Design for Productivity and Quality in Research & Development, March 17-19
- Chemometric Techniques for Quantitative Analysis, March 19

General Chemistry

- Survey of Flavor Science, March 17-18

Organic/Physical Chemistry

- Dispersions in Liquids: Suspensions, Emulsions, and Foams, March 17-18

Polymer Chemistry

- Polymeric Science and Technology, March 17-18

Professional Development

- Effective Science Communication: How to Use Storytelling and Other Delivery Techniques to Successfully Discuss Your Work with the Public and Colleagues in Unrelated Fields, March 18

2018 ACS Leadership Development System Course Offerings

Whether you are a manager, experienced professional, or new member of the workforce, we invite you to attend an ACS Leadership Development System® course held at the ACS National Meeting. The following four-hour facilitated courses have a deposit of $50 each (refunded after attendance) for ACS members and $300 fee each for nonmembers. Register for these courses when you register for the meeting. For more information and full course description, visit www.acs.org/leadershipdevelopment.

Coaching and Feedback

- March 18, 2018, 1:00 PM to 5:00 PM
  Learn how to increase performance, expand the skills of your team, encourage creativity and improve the morale of team members.

Developing Communication Strategies

- March 19, 2018, 8:00 AM to 12:00 PM

  Develop and practice your own effective communication strategy and discover how communication can make your goals possible.

Engaging and Motivating Volunteers

- March 19, 2018, 1:00 PM to 5:00 PM

  Learn practical tools to engage volunteers and to ensure successful and professional rewarding assignments, for the purpose of encouraging volunteer participation in future assignments.

Strategic Planning

- March 20, 2018, 8:00 AM to 12:00 PM

  Improve your understanding of the planning process and take advantage of the opportunity to develop your own strategic plan that aligns with the ACS Board of Director's strategic goals.

Leading without Authority

- March 20, 2018, 1:00 PM to 5:00 PM

  Learn how to gain cooperation without formal authority and motivate others to accomplish important goals.

Ticketed Social and Special Events

Organizers have planned a variety of social and special events that will take place during the meeting. Event participation is open to all interested meeting attendees. View an updated listing of social and special events, including event locations, at www.acs.org/nationalmeeting.

The following social events require a ticket, which can be purchased in the Attendee Registration Office, Lobby A in the Convention Center Rivergate Ballroom. Tickets will remain on sale until the evening before the event, if available. All tickets are sold on a first-come, first-served basis.

ACS 255th NATIONAL MEETING TICKETED EVENTS

Sunday, March 18

CHED Chemistry Educators Luncheon	$45.00	12:00 PM – 1:00 PM	Marriott Convention Center	Blaine Kern C/D
CTA Awards Luncheon	$45.00	1:00 PM – 3:00 PM	Hilton Riverside	Compass Room
Woman Chemists of Color Networking Event	No Charge	3:00 PM – 4:30 PM	Hilton Riverside	River Room
IAC Networking Globally: Education	No Charge	4:00 PM – 5:30 PM	Hilton Riverside	Windsor Room
IAC International Welcome Reception	No Charge	5:30 PM – 7:30 PM	Hilton Riverside	St. Charles Ballroom

Monday, March 19

YCC 5K Fun Run/Guided Tour (regular)	$30.00	6:45 AM - 9:00 AM	New Orleans Morial Convention Center	
YCC 5K Fun Run/Guided Tour (student)	$15.00	6:45 AM - 9:00 AM	New Orleans Morial Convention Center	
WCC WICE Breakfast (regular)	$40.00	7:30 AM – 9:00 AM	Hilton Riverside	St. James Ballroom
WCC WICE Breakfast (student)	$25.00	7:30 AM – 9:00 AM	Hilton Riverside	St. James Ballroom
CMA Luncheon (regular)	$50.00	11:30 AM – 1:30 PM	Hilton Riverside	St. James Ballroom
CMA Luncheon (student)	$25.00	11:30 AM – 1:30 PM	Hilton Riverside	St. James Ballroom
ACS/YCC Cocktail Party	No Charge	4:30PM - 6:30PM	Mardi Gras World	1380 Port of New Orleans Place
CACS Society Dinner Banquet	$40.00	7:00 PM – 9:30 PM	Hoshun Restaurant	1601 St. Charles Avenue
CARB Division Awards Dinner	$60.00	7:00 PM – 10:00 PM	Hilton Hotel, St. Charles Ballroom	333 St. Charles Avenue

Tuesday, March 20

Senior Chemist Breakfast	$20.00	7:30 AM – 9:30 AM	Hilton Riverside	Jefferson Ballroom
Univ. Of Minnesota Alumni & Friends Breakfast	$5.00	7:30 AM – 9:30 AM	Hilton Garden Inn	Magnolia Room
No Means No: How to Stop Harassment	$10.00	8:00 AM – 10:00 AM	Hilton Riverside	Grand Salon B/Section C
AFGD C4, Communicating Chemistry: Creole Cooking	$10.00	10:00 AM – 1:00 PM	Dickie Brennan's Steakhouse	716 Iberville St
CINF Division Luncheon	$30.00	12:00 PM – 1:30 PM	Hilton Garden Inn	Camillia/Gardenia Room
WCC Luncheon (regular)	$50.00	12:00 PM – 1:30 PM	Hilton Riverside	St. James Ballroom
WCC Luncheon (student)	$25.00	12:00 PM – 1:30 PM	Hilton Riverside	St. James Ballroom
COLL Division Luncheon	$45.00	12:15 PM – 1:45 PM	Hilton Garden Inn	Magnolia Room
ANYL Division Reception (regular)	$25.00	5:00 PM – 7:00 PM	Marriott Convention Center	New Levee
ANYL Division Reception (student)	$5.00	5:00 PM – 7:00 PM	Marriott Convention Center	New Levee
CELL Division Awards Banquet	$75.00	6:00 PM –10:00 PM	Pat O'Briens	600 Decatur St, 3rd Floor
ENVR Division Reception	$20.00	6:00 PM – 8:00 PM	B.B. King's Blues Club	1104 Decatur St
ENFL Division Dinner	$65.00	6:30 PM – 9:30 PM	Annunication Restaurant	1016 Annunciation St
ACS National Awards Dinner	$130.00	7:30 PM – 10:00 PM	New Orleans Marriott Canal Street	Grand Ballroom

ACS 2018 NATIONAL AWARD WINNERS

The ACS National Awards recognize individual and team accomplishments in diverse fields of chemical sciences. Award recipients traditionally receive their national award in person during the ACS awards dinner and general meeting and deliver an award address on the scientific work that is being recognized to an appropriate division.

This year's event will be held on the evening of **Tuesday, March 20, at the New Orleans Marriott Hotel.** Dinner begins at 7:30 PM, and the general meeting begins at 8:30 PM.

Geraldine L. Richmond will deliver the Priestley Medal Address at the general meeting. See Ticketed Events on page 56 for ticket information.

Several awards, such as the Arthur C. Cope Scholar Awards and the Arthur C. Cope Award, will be presented at the Arthur C. Cope Symposium in conjunction with the 256th ACS National Meeting in Boston, MA in August.

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry, sponsored by the ACS Exams Institute, **George M. Bodner**, Purdue University. Address to be presented before the Division of Chemical Education. March 19; New Orleans Marriott Convention Center; Blaine Kern C; 4:20 PM.

ACS Award for Affordable Green Chemistry, sponsored by Dow Chemical and endowed by Rohm and Haas, **Frank Gupton and David Tyler McQuade**, Virginia Commonwealth University. Address to be presented before the Division of Organic Chemistry. March 19; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 4:30 PM.

ACS Award for Computers in Chemical & Pharmaceutical Research, sponsored by the ACS Division of Computers in Chemistry, **Jürgen Bajorath**, University of Bonn, Germany, and University of Washington, Seattle. Address to be presented before the Division of Computers in Chemistry. March 20; New Orleans Marriott Convention Center; Blaine Kern D; 4:45 PM.

ACS Award for Creative Advances in Environmental Science & Technology, sponsored by the ACS Division of Environmental Chemistry and the ACS Publications journals Environmental Science and Technology and Environmental Science and Technology Letters, **Barbara J. Turpin**, University of North Carolina, Chapel Hill. Address to be presented before the Division of Environmental Chemistry. March 20; Ernest N. Morial Convention Center; Room 342; 3:50 PM.

ACS Award for Creative Invention, sponsored by ACS Corporation Associates, **Robert S. Kania**, Pfizer. Address to be presented before the Division of Medicinal Chemistry at the ACS fall national meeting in Boston, MA.

ACS Award for Creative Work in Fluorine Chemistry, sponsored by the ACS Division of Fluorine Chemistry, **Erhard Kemnitz**, Humboldt University of Berlin. Address to be presented before the Division of Fluorine Chemistry. March 19; Embassy Suites New Orleans; Fountainbleu Sec 1/2; 3:50 PM.

ACS Award for Creative Work in Synthetic Organic Chemistry, sponsored by MilliporeSigma, **Brian M. Stoltz**, California Institute of Technology. Address to be presented before the Division of Organic Chemistry. March 21; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 10:50 AM.

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry, sponsored by Strem Chemicals, **Thomas B. Rauchfuss**, University of Illinois, Urbana-Champaign. Address to be presented before the Division of Inorganic Chemistry. March 19; Ernest N. Morial Convention Center; Great Hall A; 8:15 AM.

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences, sponsored by the Camille & Henry Dreyfus Foundation, **Jani C. Ingram**, Northern Arizona University. Address to be presented before the Division of Analytical Chemistry. March 20; Ernest N. Morial Convention Center; Room 228; 8:40 AM.

ACS Award for Encouraging Women into Careers in the Chemical Sciences, sponsored by the Camille & Henry Dreyfus Foundation, **Rebecca T. Ruck**, Merck & Co.. Address to be presented before the ACS Women Chemists Committee. March 20; Hilton New Orleans Riverside; Grand Salon C Sec 13; 11:15 AM.

ACS Award for Research at an Undergraduate Institution, sponsored by Research Corporation for Science Advancement, **Joseph J. Pesek**, San Jose State University. Address to be presented before the Division of Analytical Chemistry. March 21; Ernest N. Morial Convention Center; Room 228; 3:55 PM.

ACS Award for Team Innovation, sponsored by ACS Corporation Associates, **Vladimir G. Beylin, Brian P. Chekal, Nga M. Do and Brian P. Jones**, Pfizer; **David W. Fry,** Pfizer (Retired); **Nathan D. Ide**, AbbVie; **Peter L. Toogood,** Lycera Corp. and **Hairong Zhou**, Genentech. Address to be presented before the Division of Medicinal Chemistry. March 20; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballrooms A/B; 2:15 PM.

ACS Award in Analytical Chemistry, sponsored by the Battelle Memorial Institute, **Michael Lawrence Gross**, Washington University in St Louis. Address to be presented before the Division of Analytical Chemistry. March 21; Ernest N. Morial Convention Center; Room 228; 11:10 AM.

ACS Award in Applied Polymer Science, sponsored by Eastman Chemical, **Paula T. Hammond**, Massachusetts Institute of Technology. Address to be presented before the Division of Division of Polymeric Materials: Science & Engineering and the Division of Polymer Chemistry. March 18; New Orleans Marriott Canal Street; La Galerie 6; 4:45 PM.

ACS Award in Chromatography, sponsored by MilliporeSigma, **Janusz Boleslaw Pawliszyn,** University of Waterloo, Canada. Address to be presented before the Division of Analytical Chemistry. March 20; Ernest N. Morial Convention Center; Room 228; 4:30 PM.

ACS Award in Colloid Chemistry, sponsored by Colgate-Palmolive, **Håkan Wennerström,** Lund University, Sweden. Address to be presented before the Division of Colloid & Surface Chemistry. March 20; Ernest N. Morial Convention Center; Room 242; 2:10 PM.

ACS Award in Industrial Chemistry, sponsored by the ACS Division of Industrial & Engineering Chemistry, **George P. Lahm**, DuPont. Address to be presented before the Division of Agrochemicals and the Division of Industrial & Engineering Chemistry at the ACS fall national meeting in Boston, MA.

ACS Award in Inorganic Chemistry, sponsored by Aldrich Chemical, **James M. Mayer**, Yale University. Address to be presented before the Division of Inorganic Chemistry. March 19; Ernest N. Morial Convention Center; Great Hall A; 9:20 AM.

ACS Award in Organometallic Chemistry, sponsored by the Dow Chemical Foundation, **Clifford P. Kubiak**, University of California, San Diego. Address to be presented before the Division of Inorganic Chemistry. March 19; Ernest N. Morial Convention Center; Great Hall A; 10:05 AM.

ACS Award in Polymer Chemistry, sponsored by ExxonMobil Chemical, **C. Grant Willson**, University of Texas, Austin. Address to be presented before the Division of Polymeric Materials: Science & Engineering and the Division of Polymer Chemistry. March 19; New Orleans Marriott Canal Street; La Galerie 6; 4:30 PM.

ACS Award in Pure Chemistry, sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation, **Mircea Dincă**, Massachusetts Institute of Technology. Address to be presented before the Division of Inorganic Chemistry. March 19; Ernest N. Morial Convention Center; Great Hall A; 11:05 AM.

ACS Award in Separations Science & Technology, sponsored by Waters Corp., **Massimo Morbidelli,** Swiss Federal Institute of Technology (ETH), Zurich. Address to be presented before the Division of Industrial & Engineering Chemistry. March 18; Loews New Orleans Hotel; Louisiana II; 11:05 AM.

ACS Award in Surface Chemistry, sponsored by Procter & Gamble, **Stacey F. Bent,** Stanford University. Address to be presented before the Division of Colloid & Surface Chemistry. March 20; Ernest N. Morial Convention Center; Room 242; 3:10 PM.

ACS Award in the Chemistry of Materials, sponsored by DuPont, **Elsa Reichmanis**, Georgia Institute of Technology. Address to be presented before the Division of Polymeric Materials: Science & Engineering. March 21; New Orleans Marriott Canal Street; La Galerie 6; 4:15 PM.

ACS Award in Theoretical Chemistry, sponsored by the ACS Division of Physical Chemistry, **Emily Ann Carter,** Princeton University. Address to be presented before the Division of Physical Chemistry. March 20; Ernest N. Morial Convention Center; Rooms 219/220; 2:05 PM.

Award for Volunteer Service to the American Chemical Society, sponsored by ACS, **Carol A. Duane**, D&D Consultants of Mentor. Address to be presented before the ACS ChemLuminary Awards Ceremony at the fall national meeting in Boston, MA.

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry, sponsored by the Alfred R. Bader Fund, **Alison Butler**, University of California, Santa Barbara. Address to be presented before the Division of Inorganic Division. March 19; Ernest N. Morial Convention Center; Great Hall A; 10:35 AM.

Earle B. Barnes Award for Leadership in Chemical Research Management, sponsored by the Dow Chemical Foundation, **Margaret M. Faul,** Amgen. Address to be presented before the Division of Organic Chemistry. March 18; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 11:25 AM.

Ronald Breslow Award for Achievement in Biomimetic Chemistry, sponsored by the Ronald Breslow Award Endowment, **David R. Liu,** Broad Institute, Harvard University and HHMI. Address to be presented before the Division of Biological Chemistry. March 20; Ernest N. Morial Convention Center; Room 243; 4:05 PM.

Herbert C. Brown Award for Creative Research in Synthetic Methods, sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment, **Gregory C. Fu,** California Institute of Technology. Address to be presented before the Division of Organic Chemistry. March 18; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 4:10 PM.

Alfred Burger Award in Medicinal Chemistry sponsored by Gilead Sciences, **Dennis C. Liotta**, Emory University. Address to be presented before the Division of Medicinal Chemistry. March 20; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballrooms A/B; 4:35 PM.

James Bryant Conant Award in High School Chemistry Teaching, sponsored by the Journal of Chemical Education and ChemEd X, **Brian John Kennedy**, Thomas Jefferson High School for Science & Technology, Virginia. Address to be presented before the Division of Chemical Education. March 18; New Orleans Marriott Convention Center; Blaine Kern C/D; 1:45 PM.

Arthur C. Cope Award, sponsored by the Arthur C. Cope Fund, **Steven V. Ley**, University of Cambridge, England. Address to be presented before the Division of Organic Chemistry at the ACS fall national meeting in Boston, MA.

Arthur C. Cope Scholar Awards, sponsored by the Arthur C. Cope Fund, **Emily P. Balskus**, Harvard University; **Naoto Chatani,** Osaka University, Japan; William F. DeGrado, University of California, San Francisco; **Frank Glorius**, University of Münster, Germany; **Robert Knowles**, Princeton University; **Dawei Ma**, Shanghai Institute of Organic Chemistry, Chinese Academy of Science; **Heather D. Maynard**, University of California, Los Angeles; **James Morken**, Boston College; **G. K. Surya Prakash**, University of Southern California; and **Keith Woerpel**, New York University. Address to be presented before the Division of Organic Chemistry at the ACS fall national meeting in Boston, MA.

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator, sponsored by the Pfizer Endowment Fund, **Seth B. Herzon**, Yale University. Address to be presented before the Division of Organic Chemistry. March 20; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 3:35 PM.

F. Albert Cotton Award in Synthetic Inorganic Chemistry, sponsored by the F. Albert Cotton Endowment Fund, **A. S. Borovik**, University of California, Irvine. Address to be presented before the Division of Inorganic Chemistry. March 19; Ernest N. Morial Convention Center; Great Hall A; 11:35 AM.

Peter Debye Award in Physical Chemistry, sponsored by DuPont, **Paras Nath Prasad**, State University of New York at Buffalo. Address to be presented before the Division of Physical Chemistry. March 20; Ernest N. Morial Convention Center; Rooms 219/220; 1:30 PM.

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry, sponsored by Waters Corp., **Carol Vivien Robinson**, University of Oxford, England. Address to be presented before the Division of Biological Chemistry at the ACS fall national meeting in Boston, MA.

Francis P. Garvan–John M. Olin Medal, sponsored by the Francis P. Garvan–John M. Olin Medal Endowment, **Valerie J. Kuck**, Bell Laboratories, Lucent Technologies (Retired). Address to be presented before the ACS Women Chemist Committee at the ACS fall national meeting in Boston, MA.

James T. Grady–James H. Stack Award for Interpreting Chemistry for the Public, sponsored by ACS, **Bassam Z. Shakhashiri**, University of Wisconsin, Madison. Address to be presented before the ACS Office of External Affairs and Communications at the ACS fall national meeting in Boston, MA.

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator, sponsored by the Gray Award Endowment, **Dwight S. Seferos**, University of Toronto, Canada. Address to be presented before the Division of Inorganic Chemistry. March 19; Ernest N. Morial Convention Center; Great Hall A; 8:50 AM.

Ernest Guenther Award in the Chemistry of Natural Products, sponsored by Givaudan, **David R. Williams**, Indiana University, Bloomington. Address to be presented before the Division of Organic Chemistry. March 21; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 3:55 PM.

Kathryn C. Hach Award for Entrepreneurial Success, sponsored by the Kathryn C. Hach Award Fund, **Javier García Martínez**, Rive Technology and University of Alicante, Spain. Address to be presented before the Division of Energy & Fuels. March 21; Ernest N. Morial Convention Center; Room 238; 11:35 AM.

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids, sponsored by ExxonMobil Research & Engineering, **Lawrence R. Pratt**, Tulane University. Address to be presented before the Division of Physical Chemistry. March 20; Ernest N. Morial Convention Center; Rooms 219/220; 2:40 PM.

Ralph F. Hirschmann Award in Peptide Chemistry sponsored by Merck Research Laboratories, **Lila M. Gierasch**, University of Massachusetts Amherst. Address to be presented before the Division of Biological Chemistry. March 19; Ernest N. Morial Convention Center; Room 243; 11:30 AM.

Frederic Stanley Kipping Award in Silicon Chemistry sponsored by Dow Corning**, Tamejiro Hiyama**, Chuo University, Japan. Address to be presented before the 49th Silicon Symposium, May 30-31, Edmonton, Canada.

Irving Langmuir Award in Chemical Physics sponsored by the ACS and the ACS Division of Physical Chemistry**, George W. Flynn**, Columbia University. Address to be presented before the Division of Physical Chemistry. March 20; Ernest N. Morial Convention Center; Rooms 219/220; 4:50 PM.

Josef Michl ACS Award in Photochemistry sponsored by the Josef Michl Award Endowment, **Jack Saltiel**, Florida State University. Address to be presented before the Division of Organic Chemistry. March 20; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 11:00 AM.

E. V. Murphree Award in Industrial & Engineering Chemistry, sponsored by ExxonMobil Research & Engineering, **Linda J. Broadbelt**, Northwestern University. Address to be presented before the Division of Industrial & Engineering Chemistry. March 18; Loews New Orleans Hotel; Louisiana I; 1:35 PM.

Nobel Laureate Signature Award for Graduate Education in Chemistry, sponsored by Avantor Performance Materials, **Aleksandr V. Zhukhovitskiy (student) and Jeremiah A. Johnson (preceptor)**, Massachusetts Institute of Technology . Address to be presented before the Division of Polymer Chemistry. March 20; New Orleans Marriott Canal Street; Studio 7; 11:00 AM.

James Flack Norris Award in Physical Organic Chemistry, sponsored by the ACS Northeastern Section, **Cynthia J. Burrows,** University of Utah. Address to be presented before the Division of Organic Chemistry. March 19; Ernest N. Morial Convention Center; R02; 4:00 PM.

George A. Olah Award in Hydrocarbon or Petroleum Chemistry, sponsored by the George A. Olah Award Endowment, **Oliver C. Mullins**, Schlumberger-Doll Research. Address to be presented before the Division of Energy & Fuels. March 21; Ernest N. Morial Convention Center; Room 232; 1:30 PM.

George C. Pimentel Award in Chemical Education, sponsored by Cengage Learning and the ACS Division of Chemical Education, **Pratibha Varma-Nelson**, Indiana University-Purdue University Indianapolis. Address to be presented before the Division of Chemical Education. March 20; New Orleans Marriott Convention Center; Blaine Kern A; 4:10 PM.

Priestley Medal, sponsored by ACS, **Geraldine L. Richmond**, University of Oregon. Address to be presented at the ACS National Awards Banquet Ceremony & General Meeting of the Society at the spring national meeting in New Orleans, LA.

Glenn T. Seaborg Award for Nuclear Chemistry, sponsored by the ACS Division of Nuclear Chemistry & Technology, **Suresh C. Srivastava**, Brookhaven National Laboratory. Address to be presented before the Division of Nuclear Chemistry & Technology. March 21; Embassy Suites New Orleans; Fountainbleu Sec 4; 11:15 AM.

Gabor A. Somorjai Award for Creative Research in Catalysis, sponsored by the Gabor A. and Judith K. Somorjai Endowment Fund, **David W. C. MacMillan**, Princeton University. Address to be presented before the Division of Organic Chemistry. March 19; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom C; 11:05 AM.

George & Christine Sosnovsky Award for Cancer Research, sponsored by the George & Christine Sosnovsky Endowment Fund, **Paul J. Hergenrother**, University of Illinois, Urbana-Champaign. Address to be presented before the Division of Medicinal Chemistry. March 20; Ernest N. Morial Convention Center; La Nouvelle Orleans Ballroom A/B; 1:30 PM.

E. Bright Wilson Award in Spectroscopy, sponsored by the E. Bright Wilson Endowment, **Richard J. Saykally**, University of California, Berkeley. Address to be presented before the Division of Physical Chemistry. March 20; Ernest N. Morial Convention Center; Rooms 219/220; 4:15 PM.

Ahmed Zewail Award in Ultrafast Science & Technology, sponsored by the Ahmed Zewail Endowment Fund established by Newport Corp., **Xiaoyang Zhu**, Columbia University. Address to be presented before the Division of Physical Chemistry. March 20; Ernest N. Morial Convention Center; Rooms 219/220; 3:40 PM.

National Fresenius Award, sponsored by Phi Lambda Upsilon, the National Chemistry Honor Society, **Thomas J. Maimone**, University of California, Berkeley. Address to be presented before the Division of Organic Chemistry. March 21; Ernest N. Morial Convention Center; R02; 11:10 AM.

nexus of FOOD ENERGY & WATER

STUDENT PROGRAM

March 18–19, 2018 • New Orleans, LA • Ernest N. Morial Convention Center

SUNDAY, MARCH 18, 2018

8:00 AM – 5:00 PM	**Hospitality Center** Hall D1/D2
8:30 – 11:30 AM	**Undergraduate Research Papers** *New Orleans Marriott Convention Center, Magnolia
8:30 – 9:15 AM	**Making the Most of Your First National Meeting** Hall D1/D2
9:30 – 11:00 AM	**Symposium: Where Can My Chemistry Degree Take Me?** *Cosponsored by the ACS Division of Professional Relations* Room 356
10:30 – 11:30 AM	**Graduate School: The Ins and Outs of Getting In** *Cosponsored by the ACS Division of Professional Relations and Younger Chemists Committee* Room 255–257
11:00 AM – 12:30 PM	**ChemDemo Exchange** Hall B1
12:15 – 1:30 PM	**The Graduate School Experience: What to Expect** *Cosponsored by the ACS Division of Professional Relations and Younger Chemists Committee* Room 255–257
1:00 – 5:00 PM	**Graduate School Fair** Hall E2/E3
1:30 – 3:00 PM	**Workshop: Networking 101** *Cosponsored by the ACS Division of Professional Relations and Younger Chemists Committee* Room 356–357
2:30 – 3:30 PM	**Two-Year to Four-Year College Transfer Survival Guide** Room 255–257
3:30 – 4:45 PM	**Stories from Successful ACS Student Chapter Grants** Room 255–257
7:00 – 8:30 PM	**ACS Student Chapter Awards Ceremony** Great Hall A
8:30 – 10:30 PM	**Undergraduate Social** Hall B1

MONDAY, MARCH 19, 2018

8:00 AM – 5:00 PM	**Hospitality Center** Hall D1/D2
8:30 – 11:30 AM	**Undergraduate Research Papers** *New Orleans Marriott Convention Center, Magnolia
9:00 – 10:30 AM	**Workshop: Around the World in ACS International Student Chapters: A Chapter Event Planning Exchange** Room 343
9:00 – 10:15 AM	**Workshop: Improving Scientific Communication Skills** Room 210
10:00 – 11:30 AM	**Symposium: The Chemistry that Keeps America Safe** *Cosponsored by the ACS Division of Professional Relations* Room 356–357
10:30 – 11:45 AM	**Networking Lab** *Cosponsored by the Younger Chemists Committee* Hall B1
12:00 – 2:00 PM	**Undergraduate Research Poster Session** Hall D/E
2:30 – 4:00 PM	**Eminent Scientist Lecture – Featuring Dr. Mary Jo Ondrechen, Northeastern University** Room 356–357
4:00 – 5:15 PM	**Workshop: Chemists Celebrate Earth Week** *Sponsored by the Committee on Community Activities* Hall E2/E3
5:15 – 6:15 PM	**The Fred Kavli Innovations in Chemistry Lecture** Great Hall A
8:00 – 10:00 PM	**Sci-Mix Successful Student Chapter Poster Session** Hall D/E

Find out more at **http://www.acs.org/undergradmeetinginfo**

ACS Chemistry for Life®

Visit the ACS Exposition & Career Fair!

Halls B2/C, Ernest N. Morial Convention Center

Join us for the Welcome Reception & Poster Sessions

Sunday, March 18
6:00 PM – 8:30 PM

Come back on Monday and Tuesday to continue visiting over 250 companies!

- Learn more about ACS benefits, products, services and merchandise at the ACS Booth
- Attend exhibitor workshops and demonstrations
- Network at the recharge lounge
- Meet recruiters from top companies at the Career Fair

This and much more is all happening on the newly designed ACS Expo Floor!

Monday, March 19
9:00 AM – 5:00 PM

Tuesday, March 20
9:00 AM – 5:00 PM

Caffeinate and communicate during coffee breaks!

Monday, March 19
1:00 PM – 3:00 PM

Tuesday, March 20
3:00 PM – 5:00 PM

TECHNICAL PROGRAM SUMMARY

Presidential Events — PRES

P. Dorhout, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
Water, Water Everywhere but Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water NFEW	A				
Science Cafés & Engaging the Public: Techniques for Hosting Successful Events	P				
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present *(HIST)	P	D			
Nexus of Food, Energy & Water Opening Session *(MPPG)	P				
Community Sharing of Chemical Safety Data: Yes, No, Maybe? *(CINF)		A			
Excellence in Graduate Polymer Research *(POLY)		D	DE		
State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry *(CHED)		D			
Science of Sexual Harassment *(WCC)		D			
Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web *(CINF)		P			
The Fred Kavli Innovations in Chemistry Lecture *(MPPG)		P			
The Kavli Foundation Emerging Leader in Chemistry Lecture *(MPPG)		E			
GSSPC: Finding Our Place at the Bottom *(CHED)			D		

Multidisciplinary Program Planning Group — MPPG

J. Schnoor, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Nexus of Food, Energy & Water Opening Session **	P				
Nexus of Food, Energy & Water: Adapting to Future Challenges **		P			
The Fred Kavli Innovations in Chemistry Lecture **		P			
Nano in Food, Energy & Water		P			
The Kavli Foundation Emerging Leader in Chemistry Lecture **		E			
Dreyfus Prize Symposium **			D		
Wood-Based Materials for Energy & Water *(CELL)	D	A			

Multidisciplinary Program Planning Group (continued) — MPPG

J. Schnoor, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Wearable & Implantable Sensors *(ANYL)	D	D			
Energy, Water & Food Production *(AGFD)	D				
Challenges in Determining Arsenic Compounds in Rice *(ANYL)	D				
Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present *(HIST)	P	D			
Plant Omics *(ANYL)	P				
Analytical Chemistry in the Developing World *(ANYL)	E	D	D		
Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus *(CELL)		P	D		
Science & Ethics: The Path toward Global Security in Chemicals, Energy, Food & Water *(SCHB)			P		
Comprehensive Chemical Characterization of Hydraulic Fracturing Shales, Wastes & Recycled Waste Products *(ANYL)				A	
Novel Concepts in the Role of Chemistry in the Food, Energy & Water Nexus *(ENVR)				DE	
Monitoring Pharmaceuticals & Other Pollutants in Water *(ANYL)					A

Division of Agricultural & Food Chemistry — AGFD

B. Guthrie, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
110th UMAMI Memorial Symposium: Past, Present, Future	A				
Energy, Water & Food Production **NFEW	D				
International Student Symposium	D				
Water in Foods Symposium in Honor of Louise Slade & Harry Levine NFEW	P	D	D		
General & AGFD All-Star Posters	E				
Withycombe-Charalambous Graduate Student Symposium		A			
Chemistry of Spirits		D			
Chemistry of Sex		P			
Environmental Effects on Gulf Coast Seafoods NFEW			A		
Kenneth A. Spencer Award Symposium **			D		

Division of Agricultural & Food Chemistry (continued) AGFD

B. Guthrie, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Career Trajectories for Ag & Food Chemists: Panel Discussion			P		
General Papers				D	D
Up in Smoke: Chemistry of Smoky Odors in Food & the Environment NFEW				D	
Chemistry & Applications for Cotton					A
Frontiers in Glycoscience, Bridging the Gap between Carbohydrate & Polysaccharide Chemistries *(CELL)	D	D			
Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present *(HIST)	P	D			
Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus *(CELL)		P	D		
Undergraduate Research Posters *(CHED)		P			
Nexus of Food, Energy & Water: Adapting to Future Challenges *(MPPG)		P			
Biobased Water Purification System Approaches *(CELL)			A		
Impacts of Mining & Hydraulic Fracturing on Crop & Livestock Production *(GEOC)			D		
Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium *(CHAS)				D	

Division of Agrochemicals AGRO

J. Eble, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes *(GEOC)	D			E	
Kenneth A. Spencer Award Symposium *(AGFD)			D		
Impacts of Mining & Hydraulic Fracturing on Crop & Livestock Production *(GEOC)			D		

Division of Analytical Chemistry ANYL

L. Baker, M. Bush, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Microfluidic Electrochemical Bioanalysis	A				

Division of Analytical Chemistry (continued) ANYL

L. Baker, M. Bush, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Open Resources for Automated Structure Verification & Elucidation	A				
Ultrafast Spectroscopy Meets Chemistry, Materials & Biology	D	D	D		
Wearable & Implantable Sensors ** NFEW	D	D			
Challenges in Determining Arsenic Compounds in Rice ** NFEW	D				
Active Learning in the Undergraduate Analytical Chemistry Curriculum	P				
Plant Omics ** NFEW	P				
Analytical Chemistry in the Developing World ** NFEW	E	D	D		
Analytical Division Poster Session	E				
Biomolecular, Molecular & Elemental Spectrometry with Plasma Sources		A			
Ionic Liquids: Recent Trends & Applications		D			
Analytical Chemistry of Biofuels		P			
Sci-Mix		E			
ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in Honor of Jani C. Ingram **			A		
Advancements in Biorecognition Element Discovery & Development & Its Translation into Innovative Biosensor Technologies			D		
Advances in Blood-Based Diagnostics			D		
ACS Award in Chromatography: Symposium in Honor of Janusz Pawliszyn			P		
Advances in Separations				A	
Biomedical Advances in Cancer Detection & Treatment Using Advanced Analytical Techniques				A	
Comprehensive Chemical Characterization of Hydraulic Fracturing Shales, Wastes & Recycled Waste Products ** NFEW				A	
Novel Approaches to Mass Spectrometry Imaging				A	
ACS Award in Analytical Chemistry: Symposium in Honor of Michael L. Gross				A	
Advances in Spectroscopy				P	D
Ambient Ionization & Forensic Science				P	
Forced Degradations in Pharmaceutical Industry				P	
Target-Responsive Fluorescent Probes for Detection & Diagnosis				P	

Division of Analytical Chemistry (continued) ANYL

L. Baker, M. Bush, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Joseph J. Pesek				P	
Advances in Mass Spectrometry					A
Monitoring Pharmaceuticals & Other Pollutants in Water ** NFEW					A
Advances in Electrochemistry					P
Failed Brilliance in Nanocellulose Science & Technology *(CELL)	A				
Polymer Colloids: Synthesis, Analysis, Modeling & Applications *(POLY)	D	D	DE	D	
Frontiers in Glycoscience, Bridging the Gap between Carbohydrate & Polysaccharide Chemistries *(CELL)	D	D			
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Ongoing Challenges in the Treatment of Contaminants of Emerging Concern *(ENVR)		P	D	E	
Undergraduate Research Posters *(CHED)		P			
GSSPC: Finding Our Place at the Bottom *(CHED)			D		
Inaugural Joint Symposium of the Separation Science Subdivisions *(I&EC)				D	
Advances in Bacterial (Nano)Cellulose Research *(CELL)					D

Division of Biochemical Technology BIOT

N. Tugcu, M. Antoniewicz, program chairs

InterContinental New Orleans	S	M	Tu	W	Th
BIOT Awards	A	A	AE	AE	
End-to-End Biomanufacturing	A	A	D	A	D
Downstream Processing	D	D	D	D	D
Upstream Processes	D	D	D	D	D
Biomolecular & Biophysical Processes	D	D	D	P	A
Biomedical & Emerging Technologies	P	P		D	P

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Division of Biochemical Technology (continued) BIOT

N. Tugcu, M. Antoniewicz, program chairs

InterContinental New Orleans	S	M	Tu	W	Th
BIOT Tank	E				
Sci-Mix		E			
BIOT Poster Session			E		
Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation—Anselme Payen Award Symposium in Honor of Junji Sugiyama *(CELL)	D	D	D		
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers *(POLY)		D	DE		
Undergraduate Research Posters *(CHED)		P			
WCC Rising Star Award Symposium *(WCC)			P		

Division of Biological Chemistry BIOL

S. Kelley, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Graduate Student & Postdoctoral Fellow Symposium	A			D	
Enzymes in Natural Product Biosynthesis Pathways	A				
Chemical Tools for Modulating & Imaging Biology	P				
RNA Structure & Function	P				
Current Topics	E		E		
Chemical Tools for Interrogating Biological Systems		A			
Ralph F. Hirschmann Award in Peptide Chemistry: Symposium in Honor of Lila M. Gierasch **		A			
Early Career Investigators in Biological Chemistry		P			
Goodman Award Symposium		P			
Sci-Mix		E			
ACS Chemical Biology Award Symposium			A		
Ronald Breslow Award for Achievement in Biomimetic Chemistry: Symposium in Honor of David R. Liu			P		
Midcareer Investigators in Biological Chemistry				A	
Protein Homeostasis				P	

Division of Biological Chemistry (continued) — BIOL

S. Kelley, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation—Anselme Payen Award Symposium in Honor of Junji Sugiyama *(CELL)	D	D	D		
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Biomineralization & Biocompatible Minerals *(GEOC)	D			E	
Microbially Driven Geochemical Reactions: Kinetics & Communities *(GEOC)		P	D	E	
Undergraduate Research Posters *(CHED)		P			
Chemists & Writing for Fun & Profit: Write Your Own Career *(SCHB)			A		

Division of Business Development & Management — BMGT

J. Cohen, A. DeMasi, program chairs

Hilton New Orleans Riverside	S	M	Tu	W	Th
Chemical Angel Network (CAN): Chemists Investing in Chemistry-Based Companies **	P				
Thriving in the Workplace: Nontechnical Skills That Boost Your Value **		P			
Sci-Mix		E			
Issues in Chemical Commercialization *(CHAL)		A			

Division of Carbohydrate Chemistry — CARB

S. Sucheck, program chair

Loews New Orleans	S	M	Tu	W	Th
Wolfrom Award	A				
Gin New Investigator Award	P				
Isbell Award	P				
Horton Award		A			
Advances in Molecular Recognition of Double-Helical DNA & RNA **		P	A		
Sci-Mix		E			
Recent Advances in Catalytic Carbohydrate Reaction Development **			D	A	
General Posters			E		

Division of Carbohydrate Chemistry (continued) — CARB

S. Sucheck, program chair

Loews New Orleans	S	M	Tu	W	Th
Emerging Young Investigator Symposium				D	
Frontiers in Glycoscience, Bridging the Gap between Carbohydrate & Polysaccharide Chemistries *(CELL)	D	D			
Discovery of Small Molecules Targeting RNA *(ORGN)			P		
Discovery of Small Molecules Targeting RNA: Where Are We & Where Are We Going? *(MEDI)				A	
Plant Heteropolysaccharides: Interactions within Lignocellulosics, New Modifications & Future Applications *(CELL)				D	

Division of Catalysis Science & Technology — CATL

A. Savara, program chair

Hampton Inn Convention Center	S	M	Tu	W	Th
Activation of Light ($C1$-C_4) Hydrocarbons: Theory & Experiments **	A	D	A		
Challenge & Opportunity in Lignin Valorization ** NFEW	D	A			
Electrochemical Double Layer: Modeling, Characterization & Catalysis **	D	A			
Elucidation of Mechanisms & Kinetics on Surfaces **	D	D	D	A	D
Machine Learning for Catalysis Research **	D	D			
Control of Zeolite Structure, Composition & Sites for Catalysis **	D				D
Magnetically Recoverable Catalysts **	P	P			
Operando Techniques for Catalytic & Photocatalytic Fuel Conversion Studies **		D	P		
Homogeneous Catalysis for Applied Organic Synthesis **		P	D		
Sci-Mix		E			
Toward Comprehension of Scale-Up & Multiscale Modeling of Catalysts **			A	D	
Catalytic Conversion of Biomass-Derived Molecules to Chemicals & Fuels **			D	D	D

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Division of Catalysis Science & Technology (continued) — CATL

A. Savara, program chair

Hampton Inn Convention Center	S	M	Tu	W	Th
Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in Situ & Operando Methods **			D	D	
R&D in the Chemical Catalysis for Bioenergy Consortium **			P	D	
General Catalysis			E		D
New Techniques & Applications of Magnetic Resonance Methods in Heterogeneous Catalysis				D	P
Unconventional Catalysis Targeting Stable Molecules ** NFEW				P	A
Innovative Chemistry & Materials for Electrochemical Energy Storage *(ENFL)	D	D	D	D	
Synthetic Chemistry Addressing Challenges in Energy & the Environment *(INOR)	D				
Carbon Dioxide Conversion & Artificial Photosynthesis *(ENFL)	P	D	D		
Computational Catalyst Design for Energy Conversion & Storage *(COMP)		D	D		
ACS Award Lectures *(COLL)			P		

Division of Cellulose & Renewable Materials — CELL

M. Roman, program chair

Loews New Orleans	S	M	Tu	W	Th
Failed Brilliance in Nanocellulose Science & Technology **	A				
Wood-Based Materials for Energy & Water ** NFEW	D	A			
Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation—Anselme Payen Award Symposium in Honor of Junji Sugiyama **	D	D	D		
Frontiers in Glycoscience, Bridging the Gap between Carbohydrate & Polysaccharide Chemistries **	D	D			
New Horizons in Sustainable Materials	D				
Assembly & Colloidal Interactions of Cellulose Nanocrystals **	P	D			
General Posters	E				
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Rafael Luque **		A			
Lignin: From Fundamentals to New Materials & Applications **		P	D	D	D

Division of Cellulose & Renewable Materials (continued) — CELL

M. Roman, program chair

Loews New Orleans	S	M	Tu	W	Th
Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus ** NFEW		P	D		
Sci-Mix		E			
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Ning Yan **			A		
Biobased Water Purification System Approaches ** NFEW			A		
Functional Structures from Wood-Based Materials **			P	D	D
Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems **			P	D	D
Biobased Gels & Porous Materials **				D	D
Plant Heteropolysaccharides: Interactions within Lignocellulosics, New Modifications & Future Applications **				D	
Advances in Bacterial (Nano)Cellulose Research **					D
Bioenergy & Biobased Chemicals *(ENFL)	D			D	
Energy, Water & Food Production *(AGFD)	D				
Plant Omics *(ANYL)	P				
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Fengqi You *(I&EC)		P			

Division of Chemical Education — CHED

C. Gauthier, A. Marsh, N. Snyder, program chairs

New Orleans Marriott Convention Center	S	M	Tu	W	Th
Research in Chemistry Education	A	A	A	A	A
Strategies Promoting Success of Two-Year College Students	A				
Using Light, Color & Spectroscopy to Increase Student Engagement in the Laboratory	A				
Undergraduate Research Papers	D	D			
Citizens First! **	D				
Chemistry Teachers Day Program ** NFEW	D				
NMR Spectroscopy in the Undergraduate Curriculum	D				
Chemistry Education Research: Graduate Student Research Forum	D				

Division of Chemical Education (continued) CHED

C. Gauthier, A. Marsh, N. Snyder, program chairs

New Orleans Marriott Convention Center	S	M	Tu	W	Th
Process-Oriented Guided Inquiry Learning (POGIL)	P				
Green Chemistry Student Chapters: Stories of Success	P				
Perspectives on Climate Change Literacy & Education: Local to International **	P				
General Posters	E				
ACS-CEI Award for Incorporating Sustainability into Chemical Education **		A			
International Perspectives of Chemistry Education Teaching & Practice		A			
Active Learning in the General Chemistry Curriculum		D	D		
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry		D			
State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry		D			
Curricular Innovations in Undergraduate Chemical Education Impacted by NSF		D			
General Papers		P	P	P	A
Undergraduate Research Posters **		P			
US-Cuba Collaborations in Chemical Education		P			
Successful Student Chapters		E			
STRETCH Your Students' Minds by Using Materials To Engineer Ideas about Water, Food & Energy in the Chemistry Classroom NFEW		E			
Sci-Mix		E			
Chemistry Learning & Math Learning: Which Is the Cart & Which Is the Horse?			A		
Advancing Undergraduate Research in Chemistry: Best Practices & New Innovations			D	D	
George C. Pimentel Award in Chemical Education **			D		
GSSPC: Finding Our Place at the Bottom **			D		

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Division of Chemical Education (continued) CHED

C. Gauthier, A. Marsh, N. Snyder, program chairs

New Orleans Marriott Convention Center	S	M	Tu	W	Th
Green Chemistry Theory & Practice: Food, Energy & Water Sustainability ** NFEW			D		
Statistics & Data Management in the Chemistry Curriculum			P		
Research on Learning in the Laboratory				A	
Science Communication: Engaging Science Students, Scientists & Nonscientists through Modern Communication Modes				A	
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment **				D	A
Persistence in STEM: What Can We Do To Support Students?				D	A
Engaging Students in Physical Chemistry				D	
There's an App for That!				P	
Eye Tracking Research in Chemistry Education				P	
Chemistry Safety in the Classroom: Best Practices & Learning Experience					A
Online & Upward: Improving Online Education To Increase Chemistry's Global Reach NFEW					A
Using Videos in Teaching					A
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present *(HIST)	P	D			
Integrating Polymer Science in the Curriculum *(POLY)		A	E		
Environmental Chemistry Undergraduate Education in the Classroom, Laboratory & Beyond *(ENVR)		A		E	
Implementing ACS Safety Education Guidelines *(CHAS)		P			
Chemical Information Literacy: Innovation, Collaboration & Assessment *(CINF)			D		
Undergraduate Research in Polymer Science *(POLY)			DE		
Chemistry Students at the Nexus: REU Award Winners *(PROF)			P		
WCC Rising Star Award Symposium *(WCC)			P		

Division of Chemical Health & Safety — CHAS

D. Decker, J. Pickel, program chairs

Hilton New Orleans Riverside	S	M	Tu	W	Th
Ask Dr. Safety: Integrating Research & Safety **	P				
Women in Cannabis: Shaping an Emerging Industry **		A			
Implementing ACS Safety Education Guidelines **		P			
Sci-Mix		E			
Water Supply Safety **NFEW			A		
Formulation of Cannabis Products: More than Just THC & CBD			P		
Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium **				D	
Biobased Water Purification System Approaches *(CELL)			A		
Science & Ethics: The Path toward Global Security in Chemicals, Energy, Food & Water *(SCHB)			P		
Evolving Chemical Hazard Evaluation Strategies To Address Compliance under the New Toxic Substances Control Act (TSCA) *(ENVR)			P		
Separation Science & Technology in the Medical Cannabis & Hemp Industry *(I&EC)					A

Division of Chemical Information — CINF

E. Alvaro, R. Bienstock, program chairs

New Orleans Marriott Convention Center	S	M	Tu	W	Th
Drug Discovery: Cheminformatics Approaches **	A				
Enhance Discovery: Share Chemical Structures	D				
Fragrances, Food & Cheminformatics NFEW	P				
Community Sharing of Chemical Safety Data: Yes, No, Maybe? **		A			
Workflows & Cheminformatics		D			
Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web **		P			
Sci-Mix		E			
Chemical Information Literacy: Innovation, Collaboration & Assessment **			D		

Division of Chemical Information (continued) — CINF

E. Alvaro, R. Bienstock, program chairs

New Orleans Marriott Convention Center	S	M	Tu	W	Th
Cheminformatics Resources & Software Tools Supporting Environmental Chemistry ** NFEW			D		
General Papers				A	
Drug Design *(COMP)	A	D		D	A
Large-Scale Applied Molecular Modeling *(COMP)	D	D			
Marriage of Machine Learning, Knowledge Representation & Chemical Sciences *(COMP)	D	D			
Machine Learning for Catalysis Research *(CATL)	D	D			
Computational Catalyst Design for Energy Conversion & Storage *(COMP)		D	D		
Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation *(COMP)		D	D		
ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of Jürgen Bajorath *(COMP)			D		
Structure-Based Drug Design for GPCRs *(COMP)				D	

Division of Chemistry & the Law — CHAL

K. Bianco, J. Kennedy, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions	P				
Issues in Chemical Commercialization **		A			
Update on Patent Eligibility: Are Things Getting Better for Patent Applicants?		P			
Sci-Mix		E			
Legal Issues for Chemical Companies in the Food, Energy & Water Industries *(SCHB)	P				
Evolving Chemical Hazard Evaluation Strategies To Address Compliance under the New Toxic Substances Control Act (TSCA) *(ENVR)			P		
Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium *(CHAS)				D	

Division of Colloid & Surface Chemistry — COLL

R. Nagarajan, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Basic Research in Colloids, Surfactants & Nanomaterials	A			D	A
Nanomaterials	D	D	A	A	
Biomembrane Synthesis, Structure, Mechanics & Dynamics	D	D	A	D	A
Colloidal Nanoparticle Synthesis & Assembly	D	D	A	D	A
Chemistry of Molecular Electronics **	D	D	A		
ACS Award in Surface Chemistry: Symposium in Honor of Stacey F. Bent **	D	D	A		
Fundamental Studies of Mechanochemical & Tribochemical Processes at Interfaces	D	D			
Biomaterials & Biointerfaces	D		A	D	A
Nanoparticle Biomolecule Corona: From Fundamentals to Applications	D				
Surface Chemistry	P	D		D	A
Fundamental Research in Colloids, Surfaces & Nanomaterials NFEW	E				
ACS Award in Colloid Chemistry: Symposium in Honor of Håkan Wennerström		D	A		
2018 Priestley Medalist: Symposium in Honor of Geraldine Richmond		D			
Sci-Mix		E			
Solubility of Colloids in Different Solvents			A	A	
Recent Advances in Particulate & Colloid Materials for Biomedical Applications			A	D	A
ACS Award Lectures **			P		
Fundamentals & Applications of Emulsions at Nonstandard Conditions				A	
Sol-Gel in Nanotechnology: Theory, Synthesis, Characterization & Applications				P	
Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski *(GEOC)	D	A		E	
Physical Chemistry of Ionic Liquids *(PHYS)	D	D	A	D	D

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Division of Colloid & Surface Chemistry (continued) — COLL

R. Nagarajan, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Elucidation of Mechanisms & Kinetics on Surfaces *(CATL)	D	D	D	A	D
Polymer Colloids: Synthesis, Analysis, Modeling & Applications *(POLY)	D	D	DE	D	
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Assembly & Colloidal Interactions of Cellulose Nanocrystals *(CELL)	P	D			
Magnetically Recoverable Catalysts *(CATL)	P	P			
GSSPC: Finding Our Place at the Bottom *(CHED)			D		
Functional Structures from Wood-Based Materials *(CELL)			P	D	D
WCC Rising Star Award Symposium *(WCC)			P		
Adaptive Nanogels *(POLY)			PE	D	D
Biobased Gels & Porous Materials *(CELL)				D	D

Division of Computers in Chemistry — COMP

H. Woodcock, M. Feig, J. Shen, program chairs

New Orleans Marriott Convention Center	S	M	Tu	W	Th
Drug Design **	A	D		D	A
Large-Scale Applied Molecular Modeling **	D	D			
Marriage of Machine Learning, Knowledge Representation & Chemical Sciences **	D	D			
Molecular Mechanics	D			D	A
Computational Studies of Water	D				
Undergraduate Research & COMP Career Roundtable	P				
Computational Catalyst Design for Energy Conversion & Storage ** NFEW		D	D		
Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation ** NFEW		D	D		
Sci-Mix		E			
Molecular Mechanics: Computational Studies of Transmembrane Proteins			A		
ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of Jürgen Bajorath **			D		

Division of Computers in Chemistry (continued) COMP

H. Woodcock, M. Feig, J. Shen, program chairs

New Orleans Marriott Convention Center	S	M	Tu	W	Th
Quantum Mechanics			P	D	A
Chemical Computing Group Graduate Student Travel Awards			E		
COMP Poster Session			E		
NVIDIA GPU Award			E		
OpenEye Outstanding Junior Faculty Award			E		
Wiley Computers in Chemistry Outstanding Postdoc Award			E		
Material Science				D	A
Structure-Based Drug Design for GPCRs **				D	
Drug Discovery: Cheminformatics Approaches *(CINF)	A				
Electrochemical Double Layer: Modeling, Characterization & Catalysis *(CATL)	D	A			
Adventures in Density Functional Theory *(PHYS)	D	D	A	D	D
Quantum Chemical Program Development in a Modern Computer & Programming Environment *(PHYS)	D	D	A	D	
Polymer Colloids: Synthesis, Analysis, Modeling & Applications *(POLY)	D	D	DE	D	
Machine Learning for Catalysis Research *(CATL)	D	D			
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Carbon Dioxide Conversion & Artificial Photosynthesis *(ENFL)	P	D	D		
Undergraduate Research Posters *(CHED)		P			
Toward Comprehension of Scale-Up & Multiscale Modeling of Catalysts *(CATL)			A	D	
Cheminformatics Resources & Software Tools Supporting Environmental Chemistry *(CINF)			D		

Division of Energy & Fuels ENFL

J. Liu, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Remediation of Wastewater from Energy Usage NFEW	A				
Innovative Chemistry & Materials for Electrochemical Energy Storage ** NFEW	D	D	D	D	
Bioenergy & Biobased Chemicals **NFEW	D			D	

Division of Energy & Fuels (continued) ENFL

J. Liu, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Advanced Analytical Techniques for Determination of Minor & Trace Elements in Petroleum Value Chain	D				
Materials & Processes for Solar Energy Conversion & Utilization NFEW	D				
Natural Gas Catalysis NFEW	D				
Carbon Dioxide Conversion & Artificial Photosynthesis ** NFEW	P	D	D		
Shale Gas Extraction, Conversion & Utilization NFEW	P	D			
ENFL Plenary: Reaction Mechanisms in Novel Energy & Fuel Conversion Systems		A			
Hydrogen Energy: Production, Storage & Application NFEW		D	D	D	
Issues & Challenges Related to Heavy, Light & Shale Oil Production & Processing NFEW		D	D		
Road Map & Policy of Energy & Fuels NFEW		DE	D	DE	
Sci-Mix		E			
Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of Javier García-Martínez			D	D	
ENFL Distinguished Researcher Award: Symposium in Honor of Joe D. Allison NFEW			D		
Chemistry: The Heart of Food, Energy & Water			E		
X-ray & Neutron Scattering in Energy Technologies				D	A
George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Oliver C. Mullins				D	
Alternative & Traditional Energy Resources & Energy Efficiency NFEW					A
Electrochemistry in Fuel Cells & Flexible Fuels NFEW					A
Activation of Light (C1-C 4) Hydrocarbons: Theory & Experiments *(CATL)	A	D	A		
Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski *(GEOC)	D	A		E	
Wood-Based Materials for Energy & Water *(CELL)	D	A			
Challenge & Opportunity in Lignin Valorization *(CATL)	D	A			
Electrochemical Double Layer: Modeling, Characterization & Catalysis *(CATL)	D	A			

Division of Energy & Fuels (continued) — ENFL

J. Liu, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Magnetically Recoverable Catalysts *(CATL)	P	P			
OperandoTechniques for Catalytic & Photocatalytic Fuel Conversion Studies *(CATL)		D	P		
Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus *(CELL)		P	D		
Nexus of Food, Energy & Water: Adapting to Future Challenges *(MPPG)		P			
Toward Comprehension of Scale-Up & Multiscale Modeling of Catalysts *(CATL)			A	D	
Catalytic Conversion of Biomass-Derived Molecules to Chemicals & Fuels *(CATL)			D	D	D
R&D in the Chemical Catalysis for Bioenergy Consortium *(CATL)			P	D	
Unconventional Catalysis Targeting Stable Molecules *(CATL)				P	A

Division of Environmental Chemistry — ENVR

S. Obare, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Agro-Environmental & Energy Applications of Biochar/Hydrochar	D	A		E	
Physics & Chemistry of Water Treatment: Symposium in Honor of Professor Desmond F. Lawler	D	D	A	E	
Novel Membrane-Based Technology for Water Purification & Desalination	D	D		E	
Aquatic Photochemistry	D	D		E	
Antibiotics & Antimicrobial Resistance: Developing Solutions To Address the Connectivity between Air, Food, Water & Soil NFEW	D			E	
Chemistry of Drinking Water Distribution Systems & Infrastructure	D			E	
Advances in the Transformations, Implications & Metrology of Carbonaceous Nanomaterials in the Environment	D				
Environmental Chemistry Undergraduate Education in the Classroom, Laboratory & Beyond **		A		E	
Innovative Chemical & Material Approaches for Sustainable Water Purification **		D	D	AE	

Division of Environmental Chemistry (continued) — ENVR

S. Obare, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Shaping Activity through Structural Modification: From Small Molecules to Nanoparticles: A Symposium in Honor of Professor Bing Yan		D	D	E	
Ongoing Challenges in the Treatment of Contaminants of Emerging Concern **		P	D	E	
Redox & Interfacial Dynamics among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients **		P	D	E	
Sci-Mix		E			
From Sewage to Sustainable Energy: Potential Pollution Issues from Production & Application Pathways			A	E	
Great Achievements in Environmental Science & Technology			A		
ACS Award Symposium for Creative Advances in Environmental Science & Technology **			P		
Evolving Chemical Hazard Evaluation Strategies To Address Compliance under the New Toxic Substances Control Act (TSCA) **			P		
Science & Its Perception: Climate Change, Nicotine, Pollution & Other Emerging Topics in the Crosshair **			P		
Advances & Applications in Water Sensing Technologies for Drinking Water & Agri-Tech Research				A	
Approaches To Fill Data Gaps for Chemical Sources of Risk				AE	
Advances in Understanding of Sorptive & Reactive Properties of Pyrogenic Carbonaceous Matter (PCM) in the Environment				DE	A
Accurate Mass/High-Resolution Mass Spectrometry for Environmental Monitoring & Remediation				DE	D
Current State of Environmental Contamination Research: Theory & Experiment **				DE	D

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Division of Environmental Chemistry (continued)

ENVR

S. Obare, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Novel Concepts in the Role of Chemistry in the Food, Energy & Water Nexus ** NFEW				DE	
Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery **				PE	D
Water-Use Optimization: Water Quality, Reuse & Treatment				PE	D
Contaminants in Water Sources Impacted by FEW Systems: Emerging Challenges & Opportunities NFEW				PE	
Green Chemistry & the Environment **				E	A
General Posters				E	
Nutrient Management & Water/ Wastewater Treatment through Biomass Production in Aquatic & Terrestrial Ecosystems					A
Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski *(GEOC)	D	A		E	
Wood-Based Materials for Energy & Water *(CELL)	D	A			
Challenge & Opportunity in Lignin Valorization *(CATL)	D	A			
Elucidation of Mechanisms & Kinetics on Surfaces *(CATL)	D	D	D	A	D
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Biomineralization & Biocompatible Minerals *(GEOC)	D			E	
Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes *(GEOC)	D			E	
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Rafael Luque *(CELL)		A			
ACS-CEI Award for Incorporating Sustainability into Chemical Education *(CHED)		A			
Mineral-Water Interface Geochemistry & Modeling at the Laboratory & Field Scales: Symposium in Honor of James A. Davis *(GEOC)		D	A	E	
Contaminated Site Remediation through Microbial, Geological & Chemical Processes *(GEOC)		D		E	
Lignin: From Fundamentals to New Materials & Applications *(CELL)		P	D	D	D

Division of Environmental Chemistry (continued)

ENVR

S. Obare, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Microbially Driven Geochemical Reactions: Kinetics & Communities *(GEOC)		P	D	E	
Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus *(CELL)		P	D		
Undergraduate Research Posters *(CHED)		P			
Nexus of Food, Energy & Water: Adapting to Future Challenges *(MPPG)		P			
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Ning Yan *(CELL)			A		
Biobased Water Purification System Approaches *(CELL)			A		
Water Supply Safety *(CHAS)			A		
Catalytic Conversion of Biomass-Derived Molecules to Chemicals & Fuels *(CATL)			D	D	D
Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in Situ & Operando Methods *(CATL)			D	D	
Cheminformatics Resources & Software Tools Supporting Environmental Chemistry *(CINF)			D		
GSSPC: Finding Our Place at the Bottom *(CHED)			D		
Impacts of Mining & Hydraulic Fracturing on Crop & Livestock Production *(GEOC)			D		
Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems *(CELL)			P	D	D
R&D in the Chemical Catalysis for Bioenergy Consortium *(CATL)			P	D	
Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments *(GEOC)			P	DE	D
Manganese Oxides: Their Formation, Structure, Reactivity & Applications *(GEOC)				DE	D
Unconventional Catalysis Targeting Stable Molecules *(CATL)				P	A
Forensic Geochemistry *(GEOC)				PE	
Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface *(GEOC)				E	D

Division of Fluorine Chemistry — FLUO

N. Vasdev, program chair

Embassy Suites	S	M	Tu	W	Th
ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Erhard Kemnitz	D	D	D		
Sci-Mix		E			
Radiopharmaceutical Chemistry **			E	D	D

Division of Geochemistry — GEOC

W. Burgos, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski ** NFEW	D	A		E	
Biomineralization & Biocompatible Minerals **	D			E	
Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes ** NFEW	D			E	
Mineral-Water Interface Geochemistry & Modeling at the Laboratory & Field Scales: Symposium in Honor of James A. Davis **NFEW		D	A	E	
Contaminated Site Remediation through Microbial, Geological & Chemical Processes **		D		E	
Microbially Driven Geochemical Reactions: Kinetics & Communities **		P	D	E	
Impacts of Mining & Hydraulic Fracturing on Crop & Livestock Production ** NFEW			D		
Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments ** NFEW			P	DE	D
Manganese Oxides: Their Formation, Structure, Reactivity & Applications **				DE	D
Forensic Geochemistry **				PE	
Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface **				E	D
General Geochemistry NFEW				E	

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Division of Geochemistry (continued) — GEOC

W. Burgos, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Energy, Water & Food Production *(AGFD)	D				
Carbon Dioxide Conversion & Artificial Photosynthesis *(ENFL)	P	D	D		
Redox & Interfacial Dynamics among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients *(ENVR)		P	D	E	
Undergraduate Research Posters *(CHED)		P			

Division of the History of Chemistry — HIST

N. Tsarevsky, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
Tutorial & General Papers	A			A	
Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present ** NFEW	P	D			
Sci-Mix		E			
HIST Award Symposium Honoring Jeffrey I. Seeman			D		
Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web *(CINF)		P			
Tales of Chemistry & Cocktails *(YCC)		P			

Division of Industrial & Engineering Chemistry — I&EC

C. Abney, program chair

Loews New Orleans	S	M	Tu	W	Th
ACS Award in Separations Science & Technology: Symposium in Honor of Massimo Morbidelli	A				
E. V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Linda J. Broadbelt **	D	A			
I&EC Fellow: Symposium in Honor of Yong Wang	D				
I&EC International Fellow: Symposium in Honor of Shahidah Mohd Shariff	P				
I&EC Early Career Fellow: Symposium in Honor of Beata Kilos		D	D		

Division of Industrial & Engineering Chemistry (continued) I&EC

C. Abney, program chair

Loews New Orleans	S	M	Tu	W	Th
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Fengqi You **		P			
Sci-Mix		E			
I&EC Fellow: Symposium in Honor of Dave Mackowiak: ACTP			A		
Water Purification for a Sustainable Future NFEW			P		
General Posters			E		
General Papers				A	
Inaugural Joint Symposium of the Separation Science Subdivisions **				D	
ACS Pharma Roundtable: Innovative Green Processing Technology & Chemistry				D	
Celebrating over Four Decades of Research in Nanomaterials & Commercialization: Symposium in Honor of Kenneth Klabunde **				P	D
Separation Science & Technology in the Medical Cannabis & Hemp Industry **					A
Polymer Colloids: Synthesis, Analysis, Modeling & Applications *(POLY)	D	D	DE	D	
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Rafael Luque *(CELL)		A			
Industrial Innovations in Polymer Science *(POLY)		D			
2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Ning Yan *(CELL)			A		

Division of Inorganic Chemistry INOR

S. Koch, N. Radu, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Bioinorganic Chemistry	A		AE	A	P
Coordination Chemistry	A	P	DE	P	D
Metal-Organic Frameworks: What Are Next?	D	P	DE	A	
Chemistry of Materials	D		DE	D	D
Synthetic Chemistry Addressing Challenges in Energy & the Environment **	D				

Division of Inorganic Chemistry (continued) INOR

S. Koch, N. Radu, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
ACS Award in Pure Chemistry: Symposium in Honor of Mircea Dincă	DE	P	A		
Nitrogen Unfixation: Mechanisms & Models of Nitrification/Denitrification Reactions	DE	P			
Undergraduate Research at the Frontiers of Inorganic Chemistry	DE	P			
ACS Award in Organometallic Chemistry: Symposium in Honor of Clifford P. Kubiak	DE	P			
ACS Award in Inorganic Chemistry: Symposium in Honor of James Moers Mayer	DE	P			
Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Alison Butler **	DE	P			
Organometallic Chemistry	P	P	PE	D	D
Environmental & Energy-Related Inorganic Chemistry	PE				A
Inorganic Catalysts	E	P			A
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Andrew S. Borovik	E		D	D	
Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Dwight S. Seferos	E		D		
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of Thomas B. Rauchfuss NFEW	E		D		
Inorganic Spectroscopy	E		P		
Main Group Chemistry	E			P	A
Electrochemistry	E			P	
ACS Awards in Inorganic Chemistry: Plenary Session		A			
Lanthanide & Actinide Chemistry		P	E	P	A
Sci-Mix		E			
Solid-State Inorganic Chemistry			AE		A
Molecular Confinement Effects in Inorganic & Organic Containers			DE	A	
PCET Photocatalysis with Inorganic Molecules & Materials **			DE	D	
Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals			PE	D	
Nanoscience			E		D
Activation of Light (C1-C 4) Hydrocarbons: Theory & Experiments *(CATL)	A	D	A		

Division of Inorganic Chemistry (continued) INOR

S. Koch, N. Radu, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski *(GEOC)	D	A		E	
Challenge & Opportunity in Lignin Valorization *(CATL)	D	A			
Innovative Chemistry & Materials for Electrochemical Energy Storage *(ENFL)	D	D	D	D	
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Control of Zeolite Structure, Composition & Sites for Catalysis *(CATL)	D				D
Actinide Complexes & Nanoclusters *(NUCL)	P	D	A		
Magnetically Recoverable Catalysts *(CATL)	P	P			
Homogeneous Catalysis for Applied Organic Synthesis *(CATL)		P	D		
Undergraduate Research Posters *(CHED)		P			
Catalytic Conversion of Biomass-Derived Molecules to Chemicals & Fuels *(CATL)			D	D	D
Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in Situ & Operando Methods *(CATL)			D	D	
GSSPC: Finding Our Place at the Bottom *(CHED)			D		
R&D in the Chemical Catalysis for Bioenergy Consortium *(CATL)			P	D	
Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments *(GEOC)			P	DE	D
WCC Rising Star Award Symposium *(WCC)			P		
Radiopharmaceutical Chemistry *(FLUO)			E	D	D
Unconventional Catalysis Targeting Stable Molecules *(CATL)				P	A
Celebrating over Four Decades of Research in Nanomaterials & Commercialization: Symposium in Honor of Kenneth Klabunde *(I&EC)				P	D
Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface *(GEOC)				E	D

Division of Medicinal Chemistry MEDI

A. Stamford, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Leveraging Atropisomers in Medicinal Chemistry	A				
General Orals	D		A	P	
Medicinal Chemists' Toolbox Series: Dipole & Charge in Drug Design	P				
General Posters	E			E	
Emerging Therapeutics: Gasotransmitters		A			
Impact of Small-Molecule Breakthrough Therapies on Human Health		A			
Recent Advances in the Discovery of Deubiquitinase Inhibitors		A			
2018 MEDI Young Investigators Symposium		P			
Advancing Clinical Candidates from Phenotypic Screening		P			
Identifying Selective PI 3K Inhibitors		P			
Sci-Mix		E			
Eyeing Effective Treatment for Retinal Diseases with Small Molecules			A		
Remarkable Women of Medicinal Chemistry **			A		
Boron in Medicinal Chemistry & Chemical Biology			P		
MEDI Awards Symposium			P		
Discovery of Small Molecules Targeting RNA: Where Are We & Where Are We Going? **				A	
First Time Disclosure of Clinical Candidates				D	
Large-Scale Applied Molecular Modeling *(COMP)	D	D			
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation *(COMP)		D	D		
International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers *(POLY)		D	DE		

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Division of Medicinal Chemistry (continued) MEDI

A. Stamford, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Advances in Molecular Recognition of Double-Helical DNA & RNA *(CARB)		P	A		
Undergraduate Research Posters *(CHED)		P			
ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of Jürgen Bajorath *(COMP)			D		
Discovery of Small Molecules Targeting RNA *(ORGN)			P		
Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in Honor of Seth B. Herzon *(ORGN)			P		
Radiopharmaceutical Chemistry *(FLUO)			E	D	D
Structure-Based Drug Design for GPCRs *(COMP)				D	

Division of Nuclear Chemistry & Technology NUCL

A. Hixon, program chair

Embassy Suites	S	M	Tu	W	Th
Isotope Harvesting at Accelerator Facilities	A				
Actinide Complexes & Nanoclusters **	P	D	A		
Young Investigators in Nuclear & Radiochemistry		D			
Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of Suresh C. Srivastava			P	A	
General Topics in Nuclear Chemistry & Technology				PE	
Computational Methods for Lanthanides & Actinides: Theory & Applications				E	D
Radiopharmaceutical Chemistry *(FLUO)			E	D	D

Division of Organic Chemistry ORGN

R. Broene, S. Silverman, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in Honor of Margaret M. Faul **	A				

Division of Organic Chemistry (continued) ORGN

R. Broene, S. Silverman, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
New Reactions & Methodology	D	A	A	D	
Biologically Related Molecules & Processes	D	A	E		
Frontiers in Synthetic Organic Photochemistry	D				
Asymmetric Reactions & Syntheses	DE	A			
Metal-Mediated Reactions & Syntheses	DE				
Herbert C. Brown Award for Creative Research in Synthetic Methods: Symposium in Honor of Gregory C. Fu	P				
Photoredox Chemistry	E		D		
C–H Activation	E			D	
Successful Products & Models of Undergraduate-Based Research: Good Science, Better Scientists		A			
Materials, Devices & Switches		D	E		
Twenty Years of Organo- & Photoredox Catalysis		D			
Molecular Recognition & Self-Assembly		P	DE		
ACS Award for Affordable Green Chemistry: Symposium in Honor of B. Frank Gupton & D. Tyler McQuade		P			
At the Frontier of Stereoselective Alkene Halofunctionalization		P			
James Flack Norris Award in Physical Organic Chemistry: Symposium in Honor of Cynthia J. Burrows **		P			
Sci-Mix		E			
Complex Synthetic Chemistry with Simple Starting Materials			A		
Josef Michl ACS Award in Photochemistry: Symposium in Honor of Jack Saltiel			A		
Heterocycles & Aromatics			D	AE	
Discovery of Small Molecules Targeting RNA **			P		
Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in Honor of Seth B. Herzon **			P		
Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species			PE		
Flow Chemistry & Continuous Processes			E	P	
Chemistry of Fullerenes, Carbon Nanotubes & Graphene			E		
Nanomaterials			E		

Division of Organic Chemistry (continued) ORGN

R. Broene, S. Silverman, program chairs

Ernest N. Morial Convention Center	S	M	Tu	W	Th
ACS Award for Creative Work in Synthetic Organic Chemistry: Symposium in Honor of Brian M. Stoltz				A	
National Fresenius Award: Symposium in Honor of Thomas J. Maimone				A	
Total Synthesis of Complex Molecules				DE	
Ernest Guenther Award in the Chemistry of Natural Products: Symposium in Honor of David R. Williams				P	
Peptides, Proteins & Amino Acids				PE	
New Reactions & Methodology				E	
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
General Posters *(MEDI)	E			E	
Advances in Molecular Recognition of Double-Helical DNA & RNA *(CARB)		P	A		
Homogeneous Catalysis for Applied Organic Synthesis *(CATL)		P	D		
ACS Award for Encouraging Women in the Chemical Sciences *(WCC)			A		
Recent Advances in Catalytic Carbohydrate Reaction Development *(CARB)			D	A	
Discovery of Small Molecules Targeting RNA: Where Are We & Where Are We Going? *(MEDI)				A	

Division of Physical Chemistry PHYS

M. Duncan, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Chirality from Molecules to Materials NFEW	D	D	A	D	A
Adventures in Density Functional Theory ** NFEW	D	D	A	D	D
Physical Chemistry of Ionic Liquids ** NFEW	D	D	A	D	D
Energy & Charge Transfer at Nanoscale Interfaces NFEW	D	D	A	D	
Quantum Chemical Program Development in a Modern Computer & Programming Environment ** NFEW	D	D	A	D	
Cold Molecules for Chemistry NFEW	D	D	A		
Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments NFEW	P	D	A	D	A

Division of Physical Chemistry (continued) PHYS

M. Duncan, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Sci-Mix		E			
PHYS Awards Symposium			P		
Understanding the Complexity of the Nano/Bio Interface with Experiments & Computations NFEW				D	D
PHYS Poster Session				E	
Activation of Light (C1-C 4) Hydrocarbons: Theory & Experiments *(CATL)	A	D	A		
Challenge & Opportunity in Lignin Valorization *(CATL)	D	A			
Electrochemical Double Layer: Modeling, Characterization & Catalysis *(CATL)	D	A			
Chemistry of Molecular Electronics *(COLL)	D	D	A		
Elucidation of Mechanisms & Kinetics on Surfaces *(CATL)	D	D	D	A	D
Marriage of Machine Learning, Knowledge Representation & Chemical Sciences *(COMP)	D	D			
Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials *(POLY)	D	P	E		
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation *(COMP)		D	D		
Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in Situ & Operando Methods *(CATL)			D	D	
GSSPC: Finding Our Place at the Bottom *(CHED)			D		
Dreyfus Prize Symposium *(MPPG)			D		
Polymer Networks: Soft Gels to Stiff Networks *(POLY)			DE	A	D
PCET Photocatalysis with Inorganic Molecules & Materials *(INOR)			DE	D	
Young Chemists & Water *(YCC)			P		
Unconventional Catalysis Targeting Stable Molecules *(CATL)				P	A

Division of Polymer Chemistry — POLY

T. Epps, B. Helms, C. Lipscomb, program chairs

New Orleans Marriott Canal Street	S	M	Tu	W	Th
Structure & Dynamics of Materials via NMR Spectroscopy	D	D	DE	D	D
Polymer Colloids: Synthesis, Analysis, Modeling & Applications **	D	D	DE	D	
Photochemistry & Polymers	D	D	E	D	D
Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials **	D	P	E		
General Topics: New Synthesis & Characterization of Polymers	D		DE	A	P
Polymer Applications & Characterization in Medical Device & Pharmaceutical Industries **	D		E		
International Symposium on Biorelated Polymers: Tutorial **	D				
Integrating Polymer Science in the Curriculum **		A	E		
Excellence in Graduate Polymer Research **		D	DE		
International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers **		D	DE		
Industrial Innovations in Polymer Science **		D			
Sci-Mix		E			
Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in Honor of Aleksandr Zhukhovitskiy & Jeremiah A. Johnson			A		
Polymer Networks: Soft Gels to Stiff Networks **			DE	A	D
Undergraduate Research in Polymer Science **			DE		
Adaptive Nanogels **			PE	D	D
International Symposium on Biorelated Polymers: Renewable Materials ** NFEW			E	D	D
Polymer Optoelectronics			E	D	D
Paul J. Flory Polymer Education Award: Symposium in Honor of Timothy P. Lodge				P	
POLY/PMSE Plenary & Awards Event **				E	
Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation—Anselme Payen Award Symposium in Honor of Junji Sugiyama *(CELL)	D	D	D		
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
ACS Award in Applied Polymer Science: Symposium in Honor of Paula T. Hammond *(PMSE)	D				

Division of Polymer Chemistry (continued) — POLY

T. Epps, B. Helms, C. Lipscomb, program chairs

New Orleans Marriott Canal Street	S	M	Tu	W	Th
Cyclic & Topologically Complex Polymers *(PMSE)	P	D	D	D	A
ACS Award in Polymer Chemistry: Symposium in Honor of C. Grant Willson *(PMSE)		D			
Lignin: From Fundamentals to New Materials & Applications *(CELL)		P	D	D	D
Undergraduate Research Posters *(CHED)		P			
Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems *(CELL)			P	D	D
Joint PMSE-POLY Poster Session *(PMSE)			E		

Division of Polymeric Materials Science & Engineering — PMSE

M. Becker, X. Jia, A. Norman, B. Olsen, C. Snyder, program chairs

New Orleans Marriott Canal Street	S	M	Tu	W	Th
General Papers: New Concepts in Polymeric Materials	A			D	A
Clay-Polymer Composites: Nanoclays & Other Natural Nanoparticles	D	D	A		
PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations **	D	D	A		
Polymers with Complex Architecture: From Synthesis to Self-Assembly	D	D	D	A	
Supramolecular Cross-Link Dynamics & Polymer Materials Mechanics	D				
Synergy between Computation & Experiment in Accelerated Materials Discovery	D				
ACS Award in Applied Polymer Science: Symposium in Honor of Paula T. Hammond **	D				

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Division of Polymeric Materials Science & Engineering (continued) PMSE

M. Becker, X. Jia, A. Norman, B. Olsen, C. Snyder, program chairs

New Orleans Marriott Canal Street	S	M	Tu	W	Th
Cyclic & Topologically Complex Polymers **	P	D	D	D	A
Third International Symposium on Polybenzoxazines: Toward Diamond Jubilee of Benzoxazine Chemistry		D	D	D	
Advances in Macromolecular Science & Engineering: Symposium in Honor of David Schiraldi		D			
ACS Award in Polymer Chemistry: Symposium in Honor of C. Grant Willson **		D			
Sci-Mix		E			
Symposium for Pan-American Science			D	A	
ACS Award in the Chemistry of Materials: Symposium in Honor of Elsa Reichmanis **			D	D	
Additive Manufacturing of Structures & Functional Devices: Materials, Methods, Models & Testing			P	D	A
Cooperative Research Award: Symposium in Honor of D. Bruce Chase & John F. Rabolt			P		
Joint PMSE-POLY Poster Session **			E		
Innovative Chemistry & Materials for Electrochemical Energy Storage *(ENFL)	D	D	D	D	
Polymer Colloids: Synthesis, Analysis, Modeling & Applications *(POLY)	D	D	DE	D	
Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials *(POLY)	D	P	E		
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Polymer Applications & Characterization in Medical Device & Pharmaceutical Industries *(POLY)	D		E		
International Symposium on Biorelated Polymers: Tutorial *(POLY)	D				
Integrating Polymer Science in the Curriculum *(POLY)		A	E		
International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers *(POLY)		D	DE		
Undergraduate Research Posters *(CHED)		P			
GSSPC: Finding Our Place at the Bottom *(CHED)			D		

Division of Polymeric Materials Science & Engineering (continued) PMSE

M. Becker, X. Jia, A. Norman, B. Olsen, C. Snyder, program chairs

New Orleans Marriott Canal Street	S	M	Tu	W	Th
Polymer Networks: Soft Gels to Stiff Networks *(POLY)			DE	A	D
Undergraduate Research in Polymer Science *(POLY)			DE		
International Symposium on Biorelated Polymers: Renewable Materials *(POLY)			E	D	D
Biobased Gels & Porous Materials *(CELL)				D	D
POLY-PMSE Plenary & Awards Event *(POLY)				E	

Division of Professional Relations PROF

R. Libby, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium **	D	P			
The Bond between Science & Disability: Forging New Capabilities for Inclusion		A			
Sci-Mix		E			
Ethics in Industry Collaborations That Work **			A		
Chemistry Students at the Nexus: REU Award Winners **			P		
Legal Issues for Chemical Companies in the Food, Energy & Water Industries *(SCHB)	P				
Starting a Successful Research Program at a PUI *(YCC)	P				
Chemical Angel Network (CAN): Chemists Investing in Chemistry-Based Companies *(BMGT)	P				
Entrepreneurs' Poster Session *(SCHB)	E				
How To Foster Diversity in the Chemical Sciences *(CMA)		A			
Public Policy in Food, Energy & Water Issues *(SCHB)		A			
Excellence in Graduate Polymer Research *(POLY)		D	DE		
Science of Sexual Harassment *(WCC)		D			
Thriving in the Workplace: Nontechnical Skills That Boost Your Value *(BMGT)		P			
Senior Chemists' Career Stories *(SCHB)		P			

Division of Professional Relations (continued) — PROF

R. Libby, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
Remarkable Women of Medicinal Chemistry *(MEDI)			A		
Chemists & Writing for Fun & Profit: Write Your Own Career *(SCHB)			A		
ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in Honor of Jani C. Ingram *(ANYL)			A		
ACS Award for Encouraging Women into Careers in the Chemical Sciences *(WCC)			A		
Science & Ethics: The Path toward Global Security in Chemicals, Energy, Food & Water *(SCHB)			P		
WCC Rising Star Award Symposium *(WCC)			P		

Division of Small Chemical Businesses — SCHB

J. Sabol, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
Legal Issues for Chemical Companies in the Food, Energy & Water Industries ** NFEW	P				
Entrepreneurs' Poster Session **	E				
Public Policy in Food, Energy & Water Issues ** NFEW		A			
Senior Chemists' Career Stories **		P			
Sci-Mix		E			
Chemists & Writing for Fun & Profit: Write Your Own Career **			A		
Science & Ethics: The Path toward Global Security in Chemicals, Energy, Food & Water ** NFEW			P		
Chemical Angel Network (CAN): Chemists Investing in Chemistry-Based Companies *(BMGT)	P				
Women in Cannabis: Shaping an Emerging Industry *(CHAS)		A			
Thriving in the Workplace: Nontechnical Skills That Boost Your Value *(BMGT)		P			
Ethics in Industry Collaborations That Work *(PROF)			A		
Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium *(CHAS)				D	

Committee on Chemical Safety — CCS

R. Stuart, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Ask Dr. Safety: Integrating Research & Safety *(CHAS)	P				
Implementing ACS Safety Education Guidelines *(CHAS)		P			
Water Supply Safety *(CHAS)			A		

Committee on Chemists with Disabilities — CWD

L. Hoffman, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			

Committee on Community Activities — CCA

M. McGinnis, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)				D	A

Committee on Divisional Activities — DAC

R. Bennett, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations *(PMSE)	D	D	A		
Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present *(HIST)	P	D			

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Committee on Environmental Improvement — C E I

C. Middlecamp, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Citizens First! *(CHED)	D				
Perspectives on Climate Change Literacy & Education: Local to International *(CHED)	P				
ACS-CEI Award for Incorporating Sustainability into Chemical Education *(CHED)		A			
Innovative Chemical & Material Approaches for Sustainable Water Purification *(ENVR)		D	D	AE	
Ongoing Challenges in the Treatment of Contaminants of Emerging Concern *(ENVR)		P	D	E	
Undergraduate Research Posters *(CHED)		P			
Green Chemistry Theory & Practice: Food, Energy & Water Sustainability *(CHED)			D		
Science & Its Perception: Climate Change, Nicotine, Pollution & Other Emerging Topics in the Crosshair *(ENVR)			P		
Current State of Environmental Contamination Research: Theory & Experiment *(ENVR)				DE	D
Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery *(ENVR)				PE	D
Green Chemistry & the Environment *(ENVR)				E	A

Committee on Local Section Activities — L S A C

J. Ritchie, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)				D	A

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Committee on Minority Affairs — C M A

J. Sarquis, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
How To Foster Diversity in the Chemical Sciences **		A			
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			

Committee on Science — COMSCI

M. Fisher, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Science & Ethics: The Path toward Global Security in Chemicals, Energy, Food & Water *(SCHB)			P		

Senior Chemists Committee — S C C

T. Beattie, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Senior Chemists' Career Stories *(SCHB)		P			

Society Committee on Education — SOCED

N. Bastian, program chair

Ernest N. Morial Convention Center	S	M	Tu	W	Th
Eminent Scientist Lecture with Dr. Mary Jo Ondrechen		P			
Chemistry Teachers Day Program *(CHED)	D				
Excellence in Graduate Polymer Research *(POLY)		D	DE		
Undergraduate Research Posters *(CHED)		P			
Polymer Networks: Soft Gels to Stiff Networks *(POLY)			DE	A	D
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)				D	A

Committee on Technician Affairs — C T A

C. Libby, program chair

Located with Primary Sponsor	S	M	Tu	W	Th
Water Supply Safety *(CHAS)			A		

Women Chemists Committee — W C C

R. Cole, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
Science of Sexual Harassment **		D			
ACS Award for Encouraging Women into Careers in the Chemical Sciences **			A		
WCC Rising Star Award Symposium **			P		
General Papers: New Concepts in Polymeric Materials *(PMSE)	A			D	A
Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in Honor of Margaret M. Faul *(ORGN)	A				
E. V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Linda J. Broadbelt *(I&EC)	D	A			
ACS Award in Surface Chemistry: Symposium in Honor of Stacey F. Bent *(COLL)	D	D	A		
Upstream Processes *(BIOT)	D	D	D	D	D
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Synthetic Chemistry Addressing Challenges in Energy & the Environment *(INOR)	D				
ACS Award in Applied Polymer Science: Symposium in Honor of Paula T. Hammond *(PMSE)	D				
Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in Honor of Alison Butler *(INOR)	DE	P			
Ralph F. Hirschmann Award in Peptide Chemistry: Symposium in Honor of Lila M. Gierasch *(BIOL)		A			
Women in Cannabis: Shaping an Emerging Industry *(CHAS)		A			
How To Foster Diversity in the Chemical Sciences *(CMA)		A			
Thriving in the Workplace: Nontechnical Skills That Boost Your Value *(BMGT)		P			
James Flack Norris Award in Physical Organic Chemistry: Symposium in Honor of Cynthia J. Burrows *(ORGN)		P			

Women Chemists Committee (continued) — W C C

R. Cole, program chair

Hilton New Orleans Riverside	S	M	Tu	W	Th
Remarkable Women of Medicinal Chemistry *(MEDI)			A		
ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in Honor of Jani C. Ingram *(ANYL)			A		
ACS Award in the Chemistry of Materials: Symposium in Honor of Elsa Reichmanis *(PMSE)			D	D	
George C. Pimentel Award in Chemical Education *(CHED)			D		
ACS Award Symposium for Creative Advances in Environmental Science & Technology *(ENVR)			P		

Younger Chemists Committee — Y C C

D. Williams, M. Brann, K. Heroux, program chairs

Hilton New Orleans Riverside	S	M	Tu	W	Th
Starting a Successful Research Program at a PUI **	P				
Molecules That Changed the World		A			
Tales of Chemistry & Cocktails ** NFEW		P			
Young Chemists & Water ** NFEW			P		
LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium *(PROF)	D	P			
Excellence in Graduate Polymer Research *(POLY)		D	DE		
Science of Sexual Harassment *(WCC)		D			
Thriving in the Workplace: Nontechnical Skills That Boost Your Value *(BMGT)		P			
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)				D	A

PRES

PRESIDENTIAL EVENTS

P. Dorhout, *Program Chair*

SUNDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon B Sec 9/12

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC
P.K. Dorhout, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 PRES 1. Global water resources: Meeting the demands of an increasing population. **E. Tratras Contis**

9:10 PRES 2. Reaching millions with clean water. **G. Allgood**

9:40 PRES 3. Meeting future water needs: Addressing the challenges of water quality and availability. **D.D. Reible**

10:10 PRES 4. Materials for water contaminant removal: Understanding chemistry to meet the challenges of cost, performance efficacy and lifetime. M. Abolhassani, **L.F. Greenlee**, S. Foster, C.S. Griggs, A.M. Herring, I. Ike, M. Duke

10:40 Concluding Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon B Sec 9/12

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC
P.J. Bonk, J.L. Maclachlan, *Organizers, Presiding*

1:30 Introductory Remarks.s

1:40 PRES 5. 7 years and counting: How the Cape Cod Science Cafe has evolved into a sustainable outreach mechanism for NESACS and Southeastern Massachusetts. **J.L. Maclachlan**, J.N. Driscoll

2:10 PRES 6. A decade of science cafes (and their higher-proof cousin). **S.P. Hickey**, **S.C. Dimaggio**

2:40 PRES 7. Pushing the envelope: Discussing charged topics at science cafes. **P.J. Bonk**

3:10 PRES 8. From science cafes at the Discovery Center, to a state-wide Tennessee STEAM Festival. **P.J. MacDougall**, **T.A. MacDougall**

3:40 PRES 9. "Brewing Chemistry" in Detroit: Maintaining a long running Science Café. **M.N. Murray**

4:10 Panel Discussion.
5:10 Concluding Remarks.

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Nexus of Food, Energy, & Water Opening Session
Sponsored by MPPG, Cosponsored by PRES

MONDAY MORNING

Community Sharing of Chemical Safety Data: Yes, No, Maybe?
Sponsored by CINF, Cosponsored by CHAS, CA and PRES‡

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

Science of Sexual Harassment

The Psychology & Sociology of Sexual Harassment

Sponsored by WCC, Cosponsored by PRES, PROF and YCC‡

Excellence in Graduate Polymer Research

Polymerization Techniques

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry
Sponsored by CHED, Cosponsored by PRES

MONDAY AFTERNOON

Science of Sexual Harassment

Working to Stop Harassment in Departments & at Meetings

Sponsored by WCC, Cosponsored by PRES, PROF and YCC‡

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web
Sponsored by CINF, Cosponsored by HIST and PRES

The Fred Kavli Innovations in Chemistry Lecture
Sponsored by MPPG, Cosponsored by PRES‡

State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry
Sponsored by CHED, Cosponsored by PRES

Excellence in Graduate Polymer Research

Synthesis & New Materials

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY EVENING

The Kavli Foundation Emerging Leader in Chemistry Lecture
Sponsored by MPPG, Cosponsored by PRES

TUESDAY MORNING

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, ENVR‡, INOR, PMSE‡ and PRES‡

Excellence in Graduate Polymer Research

Bio-Related Polymers

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY AFTERNOON

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, INOR, PHYS‡, PMSE‡ and PRES‡

Excellence in Graduate Polymer Research

New Products & Characterization

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY EVENING

Excellence in Graduate Polymer Research
Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MPPG

Multidisciplinary Program Planning Group

J. Schnoor, *Program Chair*

SUNDAY MORNING

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Challenges in Determining Arsenic Compounds in Rice
Sponsored by ANYL, Cosponsored by MPPG‡

Energy, Water & Food Production
Sponsored by AGFD, Cosponsored by CELL, GEOC and MPPG

Wearable & Implantable Sensors
Sponsored by ANYL, Cosponsored by MPPG‡

Wood-Based Materials for Energy & Water

Nanocellulose-Based Technologies

Sponsored by CELL, Cosponsored by ENFL, ENVR and MPPG

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Great Hall A

Nexus of Food, Energy, & Water Opening Session
Cosponsored by PRES
J.L. Schnoor, *Organizer, Presiding*
A.C. Collins, *Presiding*

3:00 Introductory Remarks.

3:05 MPPG 1. Transitioning world energy for all purposes to stable electricity powered by 100% wind, water, and sunlight. **M. Jacobson**

3:35 Q&A.

3:40 MPPG 2. Advanced materials and processes for energy and water. **Y.H. Hu**

4:10 Q&A.

4:15 MPPG 3. Nanoparticle technology enabling smart agriculture solutions: Nexus of food and environment. **P. Biswas**, R. Raliya, S. Dhawan

4:45 Q&A.

4:50 MPPG 4. Unconventional hydrocarbon development and water resources. **D.A. Dzombak**

5:20 Q&A.

5:25 MPPG 5. Integrating systems of water reuse and desalination: More water, less energy. **A. Childress**

5:55 Q&A.
6:00 Concluding Remarks.

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

Challenges in Determining Arsenic Compounds in Rice
Sponsored by ANYL, Cosponsored by MPPG‡

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

Energy, Water & Food Production
Sponsored by AGFD, Cosponsored by CELL, GEOC and MPPG

Plant Omics
Sponsored by ANYL, Cosponsored by

‡*Cooperative Cosponsorship*

CELL and MPPG‡

Wearable & Implantable Sensors
Sponsored by ANYL, Cosponsored by MPPG‡

Wood-Based Materials for Energy & Water

Wood-Fiber & Wood-Scaffold Based Technologies

Sponsored by CELL, Cosponsored by ENFL, ENVR and MPPG

MONDAY MORNING

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

Analytical Chemistry in the Developing World

Environmental Applications

Sponsored by ANYL, Cosponsored by MPPG‡

Wearable & Implantable Sensors
Sponsored by ANYL, Cosponsored by MPPG‡

Wood-Based Materials for Energy & Water

Wood-Based & Related Materials

Sponsored by CELL, Cosponsored by ENFL, ENVR and MPPG

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Great Hall A

The Fred Kavli Innovations in Chemistry Lecture
Cosponsored by PRES
P.K. Dorhout, *Organizer, Presiding*
A.C. Collins, *Presiding*

5:15 Introductory Remarks.

5:20 MPPG 6. Giving new life to materials for energy, the environment and medicine. **A.M. Belcher**

6:10 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 206

Nexus of Food, Energy, & Water: Adapting to Future Challenges
Cosponsored by AGFD‡, ENFL‡ and ENVR‡
D.D. Dionysiou, L. Houston, J.L. Liu, B. Park, *Organizers*
S.O. Obare, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 MPPG 7. Feeding 9 billion: A USDA perspective. **G.E. Lester**

1:30 MPPG 8. Convergence of science and technology to address nexus of food, energy, & water. **H. Chen**

1:55 MPPG 9. Sustainable planning of food-energy-water nexus through decision making tools. **X. Wang**, N. Bieber, J. Ker, N. Shah

2:20 MPPG 10. The role of food, energy, water systems (FEWS) in domestic resilience and security. **L. Alessa**, A. Kliskey, J.C. Foltz, J. Stahlman, J. Nelson

2:45 MPPG 11. Regulation of water pollution from coal ash ponds. **P.R. Robinson**

3:10 Intermission.

3:20 MPPG 12. Toward a molecular scale understanding of nutrient (re)cycling. **Y. Tang**, R. Huang, C. Fang, B. Wan

3:40 MPPG 13. Tackling challenges in catalyst design: Interdisciplinary lessons on iron-based nanomaterials for efficient water treatment and electrochemical energy conversion. **L.F. Greenlee**

4:00 MPPG 14. Role of membrane technology towards sustainability & life sciences. **M. Paul**, A. Roy, I.A. Tomlinson, S. Rosenberg, S. Jons, M. Peery, R.C. Cieslinski

4:20 MPPG 15. Phosphorus sequestration from nonpoint particulate runoff via extraction using fungal carboxylic acids: Factorial effects on recovery efficiency and extraction kinetics. **A. Mondala**, S. Shields, K. Gaviglio, Y. Arai

4:40 MPPG 16. Phosphate recognition in solution and at aqueous interfaces. **A.H. Flood**, W. Zhao, J.F. Neal, H.C. Allen

5:00 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 215

Nano in Food, Energy, & Water

P. Alivisatos, H. Atwater, J.M. Buriak, L.E. Fernandez, C. Toro, P.S. Weiss, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 MPPG 17. Optimization of organic solar cell processing parameters: Combining machine learning and experimental design. **J.M. Buriak**, B. Cao, B. Olsen, E.J. Luber

1:35 MPPG 18. Novel 2D materials for addressing water and energy challenges. **Y. Gogotsi**

2:05 MPPG 19. Nanoscale design and cryogenic electron microscopy for of energy storage. **Y. Cui**

2:35 MPPG 20. Nanocrystal inks and nanowire networks for paper solar cells, improved batteries and water purification membranes. **B.A. Korgel**

3:05 MPPG 21. Tuning coupling with plasmonic metal oxide nanocrystals. **D.J. Milliron**

3:35 MPPG 22. Nanophotonics for the terawatt solar age: New concepts for generation of electricity and fuels from sunlight. **H. Atwater**

Analytical Chemistry of Biofuels
Sponsored by ANYL, Cosponsored by MPPG‡

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

Analytical Chemistry in the Developing World

Food & Nutrition

Sponsored by ANYL, Cosponsored by MPPG‡

Wearable & Implantable Sensors
Sponsored by ANYL, Cosponsored by MPPG‡

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Value Added from Agricultural Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Great Hall A

The Kavli Foundation Emerging Leader in Chemistry Lecture
Cosponsored by PRES

P.K. Dorhout, *Organizer, Presiding*

4:00 Introductory Remarks.

4:05 MPPG 23. Transforming nanocellulose into sustainable products through surface engineering. **E.D. Cranston**

4:55 Q&A.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 206

Dreyfus Prize Symposium

Theory & Computation

Cosponsored by COMP‡, PHYS‡ and PRES
M.J. Cardillo, *Organizer*
L.E. Brus, R. N. Zare, *Presiding*

9:00 Introductory Remarks. **J. Schnoor**

9:10 Introductory Remarks.

9:15 MPPG 24. Insights from Ab initio potential energy surfaces and molecular dynamics for sustainable energy technologies. **E.A. Carter**

9:50 MPPG 25. Dynamics and mechanisms of pericyclic reactions. **K. N. Houk**

10:25 Intermission.

10:40 MPPG 26. Field-theoretic simulations: From advanced materials to quantum liquids. **G.H. Fredrickson**

11:15 MPPG 27. Metals, molecules, mixing, and mastery. **M.A. Ratner**

Analytical Chemistry in the Developing World

Applications in Medicine

Sponsored by ANYL, Cosponsored by MPPG‡

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Food, Water & Energy from Sustainable Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 206

Dreyfus Prize Symposium

Theory & Computation

Cosponsored by COMP‡, PHYS‡ and PRES

M.J. Cardillo, *Organizer*
D.G. Nocera, M.V. Tirrell, *Presiding*

2:00 MPPG 28. How to burn water with sunlight? Insights from computational chemistry. **W. Domcke**

2:35 MPPG 29. Proton-coupled electron transfer in catalysis and energy conversion. **S. Hammes-Schiffer**

3:10 Intermission.

3:25 MPPG 30. Variational sampling and renormalization theory. **R. Car**

4:00 MPPG 31. Fluctuations, entropy and rare events. **M. Parrinello**

Science & Ethics: The Path Toward Global Security in Chemicals, Energy, Food & Water
Sponsored by SCHB, Cosponsored by CHAS, COMSCI, MPPG and PROF

Analytical Chemistry in the Developing World

Technology Development

Sponsored by ANYL, Cosponsored by MPPG‡

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Biomaterials Processing

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

WEDNESDAY MORNING

Novel Concepts in the Role of Chemistry in the Food, Energy & Water Nexus
Sponsored by ENVR, Cosponsored by MPPG

Comprehensive Chemical Characterization of Hydraulic Fracturing Shales, Wastes & Recycled Waste Products
Sponsored by ANYL, Cosponsored by MPPG‡

WEDNESDAY AFTERNOON

Novel Concepts in the Role of Chemistry in the Food, Energy & Water Nexus
Sponsored by ENVR, Cosponsored by MPPG

THURSDAY MORNING

Monitoring Pharmaceuticals & Other Pollutants in Water
Sponsored by ANYL, Cosponsored by MPPG‡

‡*Cooperative Cosponsorship*

AGFD

Division of Agricultural & Food Chemistry

B. Guthrie, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Advancements in Bio-Recognition Element Discover & Development & Its Translation into Innovative Biosensor Technologies (see *ANYL*, Tue)

Enzymes in Natural Product Biosynthesis Pathways (see *BIOL*, Sun)

Fragrances, Food & Cheminformatics (see *CINF*, Sun)

Water Purification for a Sustainable Future (see *I&EC*, Tue)

Molecular Mechanics: Computational Studies of Transmembrane Proteins (see *COMP*, Tue)

Advances & Applications in Water Sensing Technologies for Drinking Water & Agri-Tech Research (see *ENVR*, Wed)

SOCIAL EVENTS:

Reception/Poster Session, 5:30 PM: Sun

AGFD Chair Reception, 6:00 PM: Tue

BUSINESS MEETINGS:

AGFD Special Topics Meeting, 12:00 PM: Sun

AGFD Future Programs Meeting, 12:00 PM: Mon

AGFD Executive Committee Meeting, 5:00 PM: Mon

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 218

110th UMAMI Memorial Symposium: Past, Present, Future

Financially supported by Ajinomoto Co., Inc
I. Edirisinghe, H. Uneyama, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 1. History of umami research on scientific literature. **S. Fukuoka**

8:35 AGFD 2. Key research in umami science. **G. Beauchamp**

9:05 AGFD 3. Beyond taste: Does umami contribute to healthier life? **H. Uneyama**

9:35 AGFD 4. Umami in the United States: A history of Americans came to fear MSG but love umami. **S. Lohman**

10:05 AGFD 5. Creation of global umami network through science communication. **K. Ninomiya**

10:35 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 217

Energy, Water & Food Production
Cosponsored by CELL, GEOC and MPPG
M. Appell, X. Fan, J.W. Finley, B. Park, J.N. Seiber, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 6. Climate change and the food, energy water nexus. **J.W. Finley**

8:30 AGFD 7. Formation of atmospheric aerosols in the presence of sulfide and amine compounds: implications for farm waste. **M.J. Nee**, J. Berlanga, P. van Rooy, D. Cocker, K. Purvis-Roberts, P.J. Silva, R. Mahmood

8:55 AGFD 8. Managing challenges of the climate-food-energy-water nexus. **S. Ahuja**

9:20 AGFD 9. Sorption characteristics of glyphosate in Australian soils. **G. Styles**, M. Rose, L. Van Zwieten, B. Follink, A. Patti

9:45 AGFD 10. Nanoparticle N-P-K fertilizers synthesized by aerosol routes for sustainable and precision agriculture. **R. Raliya**, P. Biswas

10:10 AGFD 11. Zein nanoparticles as viable delivery systems for agrochemicals. K. Ristroph, A. Prasad, E. Bodoki, C.E. Astete, A. Bodoki, **C. Sabliov**

10:35 Intermission.

10:55 AGFD 12. The role of soil properties on the transformation, fate and efficacy of nano-enabled agrochemicals in the soil system. **S. Rodrigues**, S. Lopes, T. Trindade, A. Duarte, R. Duarte, X. Gao, G.V. Lowry

11:20 AGFD 13. Withdrawn

Section C
Ernest N. Morial Convention Center
Room 216

International Student Symposium

Analytical Strategies

F. Pellati, P. Schmidberger, *Organizers*
R. Tardugno, *Organizer, Presiding*
A. Schulz, *Presiding*

8:30 Introductory Remarks.

8:35 AGFD 14. Development of an indirect competitive enzyme-linked immunosorbent assay for Matrine and analogues in agricultural samples. **J. Hao**, E. Sheng

9:05 AGFD 15. Novel benzophenone isolated from *Psidium guajava* L. leaves and its antineoplastic effects on human cancer cells. **X. Zhu**, W. Ouyang, C. Pan, Z. Gao, Y. Han, M. Song, K. Feng, Y. Cao, H. Xiao

9:35 AGFD 16. Effectiveness of commercial and homemade washing agents in removing pesticide residues on and in apples. **T. Yang**, L. He

10:05 Intermission.

10:15 AGFD 17. The chemistry of beer haze. **B. Baechler**, A. Dunkel, T. Hofmann

10:45 AGFD 18. Metabolomic profiling of saliva and pellicle samples collected from healthy and caries patients. **A. Schulz**, R. Lang, J. Behr, S. Hertel, C. Hannig, M. Hannig, T. Hofmann

11:15 Concluding Remarks.

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 218

Water in Foods Symposium in honor of Louise Slade & Harry Levine

Food Polymer Science

J.W. Finley, Y. Roos, *Organizers, Presiding*

1:00 Introductory Remarks.

1:30 AGFD 19. 37-year retrospective on Slade/Levine's 'Food Polymer Science' approach to the practice of industrial R&D, leading to U.S. patent estates based on fundamental starch science and technology. **L. Slade**, **H. Levine**

2:30 AGFD 20. Crystallization, crispness, caking and creep: The glass of water overturned. **T.P. Labuza**

3:00 Intermission.

3:10 AGFD 21. Approaches for stucture-properties-performance translation of relaxation times data around glass transition. **Y. Roos**

3:40 AGFD 22. Physical state of sugar in baked goods: Revisiting an early "Food Polymer Science" application. **J. Ubbink**, N. Salgado Lopez, K.M. Matsune, S. Amin

4:10 AGFD 23. Water induced structural hysteresis in food systems. **S. Mizrahi**

4:40 AGFD 24. Complementary tools to interpret the role of water as related to structure and functionality of cereal food products. G. Rolandelli, S. Rodriguez, M. Cueto, A. Farroni, **P. Buera**

Section B
Ernest N. Morial Convention Center
Room 217

Energy, Water & Food Production
Cosponsored by CELL, GEOC and MPPG
M. Appell, X. Fan, J.W. Finley, B. Park, J.N. Seiber, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 25. Creatine a scavenger of methylglyoxal (MGO), a potent neurotoxin: Physiological role of creatine in energy metabolism. **B. Dayal**, M.A. Lea, P. Chitkul, H. Sorkin

1:30 AGFD 26. Nexus of beer, water and energy: California lager microbrewery as a case study of embedded water and energy in the brewing process. **S. Peterson**, C. Simmons, N. Spang

1:55 Intermission.

2:15 AGFD 27. Combating citrus greening with plastic. **V.A. Piunova**, N.F. Fine Nathel, J.L. Hedrick

2:40 AGFD 28. Effects of metal oxide nanoparticles on the growth of kale. J. Vassell, A. Racelis, **Y. Mao**

3:05 AGFD 29. Paper-based nanosensors for selective detection of infected crops. **O.A. Sadik**

3:30 AGFD 30. Indigo's potential to address long-term food security in an era of global change. **J. McIntyre**

3:55 AGFD 31. Assessing agricultural intensification strategies with a sustainable agriculture matrix. **X. Zhang**

4:20 AGFD 32. Inexpensive superhydrophobic sand mulches for dryland agriculture. **A. Gallo, Jr.**, J. Reihmer, M. Mousa, M. Morton, S. Al-Mashharawi, M. McCabe, M. Tester, H. Mishra

4:45 AGFD 33. Withdrawn

5:10 Panel Discussion.

Section C
Ernest N. Morial Convention Center
Room 216

International Student Symposium

Bioactives & Cell Studies

F. Pellati, P. Schmidberger, *Organizers*
R. Tardugno, *Organizer, Presiding*
A. Schulz, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD 34. Permethrin and ivermectin modulate lipid metabolism in steatosis-induced HepG2 hepatocytes. **S. Yang**, W. Qi, S. Choi, J.M. Clark, Y. Park

1:35 AGFD 35. Investigation of the bioavailability, antioxidant and anti-inflammatory activities of carnosic acid lecithin based nano delivery system by in vitro cell models. **H. Zheng**, Q. Huang

2:05 AGFD 36. Hydrophilic modification of zein protein and its application in amorphous solid dispersions to enhance issolution of Dihydromyricetin. **H. Zhang**, **Q. Huang**

2:35 Intermission.

2:45 AGFD 37. Anti-inflammation and anti-cancer effect of polyphenols from blueberry (*Vaccinium corymbosum* L.). **C. Pan**, Z. Gao, Y. Han, H. Xiao

3:15 AGFD 38. Pickering emulsions stabilized by milled cellulose particles. **X. Lu**

3:45 Concluding Remarks.

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, PRES‡ and MPPG‡

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall E

‡*Cooperative Cosponsorship*

General & AGFD All-Star Posters

B.D. Guthrie**,** *Organizer*

5:30–7:30

AGFD 39. Multiplex and label-free screening of foodborne pathogens using surface plasmon resonance imaging. J. Chen, **B. Park**

AGFD 40. Computational studies on the excited state properties of citrinin and application in fluorescence analysis. **M. Appell**, Y. Tu, W. Bosma

AGFD 41. Traveling the world with food science. **J.V. Leland**

AGFD 42. Ion mobility mass spectrometry of *Garcinia buchananii* extracts and analysis of other *Garcinia* species. T. Hofmann, T.D. Stark, **J. Ranner**

AGFD 43. Development of a rapid high-throughput mass spectrometry-based method for the quantification of monosaccharides in food. **T. Vo**, A.G. Galermo, M. Amicucci, C.B. Lebrilla

AGFD 44. Characterization of gelation kinetics of gelatin using fluorescence spectroscopy. **A. Ciarfella**, R. Chib, M.G. Corradini, S. Ilg, C. Escusa, R.D. Ludescher

AGFD 45. Development of paper-polymer hybrid chip for multiplexed detection of foodborne pathogens. **L. Zhang**, J. Choi, X. Lu

AGFD 46. Study of volatile compounds with antifungal activity from bacteria of marine origin. **L.C. Coconubo**, F. Ramos, L. Castellanos, N. Moreno, D.C. Sinuco Leon

AGFD 47. Preparation and characterization of seed film coating adhesive for anti-dust. **D. Ku**, J. Lee, J. Lee, J. Kim, J. Shim, T. Kim

AGFD 48. Concentration and removal of phosphate from corn thin stillage using biobased flocculants and ferric chloride. **G.J. Piazza**, D.B. Johnston, R.A. Garcia

AGFD 49. Bio-based methacrylic acid via catalytic decarboxylation of itaconic and citric acids. **B.R. Moser**, R.E. Murray, J.C. Lansing

AGFD 50. Structure and compositional features of feruloylated arabinoxylan oligosaccharides isolated from rice bran fiber. **K. Takahashi**, B.J. Savary, S. Lee, N.C. Carpita

AGFD 51. Structure, composition, and oligosaccharide profiles for hemicellulosic polysaccharides isolated from rice bran fiber. **D. Kandanool**, A. Vallalpa-Arroyo, K. Takahashi, B.J. Savary, N.C. Carpita

AGFD 52. Determination of lactose in low lactose products. **J. Rohrer**, M. Aggrawal

AGFD 53. Rethinking resveratrol from red wine: The first characterization of piceatannol-*ortho*-quinone, a structural analogue of carcinogenic estradiol-3,4-quinone. **M.K. Parunyan**, J. Jensen, E. Philippas, G.G. Melikyan

AGFD 54. Effects of feeding entrapped fish oil in chemically treated protein matrix on physicochemical properties of caprine milk fat. **J.H. Lee**, B.B. Lemma, **C.R. Alfred**

AGFD 55. Quality assessment of moisture exposed almonds using chemical markers. **K. Luo**, A.E. Mitchell

AGFD 56. Extraction and quantitation of furfuryl alcohol in fluid milk and dairy powders. **M. Benoist**, B. Wherry, M. Drake

AGFD 57. Animal and human studies investigating the beneficial effects of cranberry juice on heart disease. **J.A. Vinson**

AGFD 58. Withdrawn

AGFD 59. Fatty acid and sugar composition of African walnut (*Plukenetia conophora Mull.Arg*) root bark. **O.O. Onawumi**, **P.B. Ayoola**

AGFD 60. Hydrophilic interaction chromatographic (HILIC) determination of ascorbic acid in citrus fruits and pharmaceutical formulations. R. Zuo, S. Zhou, **Y. Zuo**, Y. Deng

AGFD 61. Phenylalanine ammonia lyase activity and antioxidant properties of *Cissus sicyoides* berries. **K.S. Duffus**, A. Goldson-Barnaby

AGFD 62. Extraction and quantification of lycopene content for high performance liquid chromatography analysis using alternative solvents. **J. Noseworthy**

AGFD 63. Comparative analysis of silymarin using different extraction techniques. **D. Hlangothi**, K. Anthony, M.A. Saleh

AGFD 64. Chemical profile of *chrysanthemum morifolium* and its nutraceutical properties. **L. Yanfang**, B. Gao, L. Yu, U. Choe, H. Huang, T. Wang, L.L. Yu

AGFD 65. Determination of polyphenolic antioxidants in natural and processed foods by copper nanoparticles. **Y. Ahmadibeni**

AGFD 66. Determination of fluoride in tea using combustion ion chromatography. **H. Yang**

AGFD 67. Withdrawn

AGFD 68. Anthocyanin concentrations, antioxidant properties, and phenolic contents among commercially available acai berry supplements. **T. Beadle**, E.D. Niemeyer

AGFD 69. Influence of fatty acids on the formation of zein-based colloidal particles. **J. Zhu**, Q. Huang

AGFD 70. Yeast viability determination by smartphone camera. **A. Nilles**, D.J. Lecaptain

AGFD 71. Modification of sensory-chemical quality of lingonberry (*Vaccinium vitis-idaea)* products using polymers. **N. Kelanne**, O. Laaksonen, B. Yang, W. Yang

AGFD 72. Identification and quantification of flavor compounds in birch syrup using SPME-GC-MS. **S. Lloyd**, A. van den Berg, C.C. Grimm

AGFD 73. Honey typing by comparison of flavor compounds in floral nectars and honeys. **K. Petz**, T. Calamita, L.E. Schweitzer

AGFD 74. Effect of hot/cold cycling and air exposure on beer IBU values. J. Welbaum, **N.O. Flynn**

AGFD 75. Composition profile: A comparative study of hop varieties grown in the Midwest and Pacific Northwest of the United States. **X. Xie**, L. Gao, C. Xu

AGFD 76. Investigation of catfish marinate treatments on the degradation of off-flavor components, geosmin and 2-methylisoborneol. **J.M. Bland**, C.H. Li, K.L. Bett-Garber, C.C. Grimm, P. Bechtel

AGFD 77. Optimizing the analysis for off-flavors in fish tissue. **C.C. Grimm**, J.M. Bland, C. Li, P. Bechtel

AGFD 78. Thermal desorption with GC-MS to detect volatiles in craft beer. **A. LyVere**, D.J. Lecaptain

AGFD 79. Static headspace GC-FID/MS method for the determination and quantitation of residual solvents in natural food ingredients. **F. Al-Taher**, B.V. Nemzer

AGFD 80. Production of mushroom-glucan-gold nanorod hydrids for photothermal therapy of cancer. X. Li, **P.C. Cheung**

AGFD 81. Quantitative analysis of arsenic and cadmium in dog food. **K. Pollok**, R. Nava, B. Corporon, A.M. Bray

AGFD 82. Functional analyses on antioxidant, antitumor and hepatoprotective effects of extracts and compounds from *Cirsium japonicum* DC. **Q. Ma**

AGFD 83. Washing tomato fruit with organic acids to reduce populations of *Salmonella* and preserve fruit quality. **X. Fan**, J. Gurtler, K. Sokorai

AGFD 84. Aged catechol solutions model the chemical and biochemical properties of the aqueous cigarette tar radical. C. Lopez, A.R. Skochko, S.K. Mendez, E.A. Aleman, **K. Stone**

AGFD 85. Identification and functional analysis of the aspergillic acid gene cluster in *Aspergillus flavus*. **M. Lebar**, J. Cary, R. Majumdar, C. Carter-Wientjes, B. Mack, Q. Wei, V. Uka, S. De Saeger, J. Diana Di Manvungu

AGFD 86. Development of rapid dispersive pipette extraction method for analysis of aflatoxins and major metabolite using high performance liquid chromatography (HPLC). **H. Guan**, Q. Cai

AGFD 87. Plant cuticular waxes as renewable encapsulating matrices for phosphate fertilizers: Morphological insights into phosphate release behavior. E.M. García Carrillo, **N.B. Navarro-Guajardo**, **C. Espinoza-González**, J. Romero-García, A.S. Ledezma-Pérez, C.A. Pérez Torres, N. Pariona

AGFD 88. Sequence alignments and structural comparisons of insecticides targeting acetyl cholinesterase and their relationship to ecotoxicity/toxicity. Z. Kai, **F.H. Wu**

AGFD 89. Fate and transport of dicyandiamide (DCD) and its nitrification inhibition in agricultural soils. **S. Li**, R. Li, G. Chen

AGFD 90. Chemistry of plant root signaling compounds with importance for the plant-associated microbiome and disease resistance. **K. Hooshmand**, E.N. Kudjordjie, R. Sapkota, M. Nicolaisen, I.S. Fomsgaard

AGFD 91. Importance of animal production to produce energy. **T. Akinmusire**

AGFD 92. Water and energy in agriculture. **T. Akinmusire**

AGFD 93. Adduct formation from chlorinated benzonitrile pesticides and DNA in plants. **M. Byron**, D.W. Boerth

AGFD 94. Molecular and immunological characterization of recombinant termite (*Coptotermes formosanus*) arginine kinase. **C.P. Mattison**, A. Tungtrongchitr

AGFD 95. Screening and health risk of organic micro-pollutants in rural groundwater of China. **X. Li**, T. Tian, X. Shang, Q. Xie, J. Chen, K. Kadokami

AGFD 96. New insights into kinetics and dynamics of initial stages of bacterial adhesion onto surfaces mimicking food crops. **J. Oh**, Y. Yegin, L. Cisneros-Zevallos, M. Akbulut

AGFD 97. Determination of inorganic anions in wastewater using capillary ion chromatography. **H. Yang**

AGFD 98. Chemical space of in-use and banned pesticides. **K. Martinez Mayorga**, D. Chavez-Gomez, F. Cortes-Guzman

AGFD 99. Analysis of volatile organic compounds from *M. phaseolina* fungi infected sweet potatoes. **C.U. Gamlath Mohottige**, J. She, T. Mlsna, R. Baird, R. Bigham

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 216

Water in Foods Symposium in honor of Louise Slade & Harry Levine

Water Plasticization

J.W. Finley, Y. Roos, *Organizers*

Y. Roos, *Organizer, Presiding*
T.P. Labuza, *Presiding*

8:00 AGFD 100. Impact of sucrose and water contents on macroscopic structure and stability of cereal based products: Thermodynamic versus dynamic. S. Masavang, C. Loupiac, P. Bodart, G. Roudaut, **D. Champion**

8:30 AGFD 101. Sucrose crystallization and the state diagram: A review. **R.W. Hartel**, K. Payne

9:00 AGFD 102. Fundmentals and consequences of food ingredient architecture and water-solid interactions. **L.J. Mauer**

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9:30 AGFD 103. Plasticization and antiplasticization in amorphous carbohydrates: A structural interpretation. **J. Ubbink**

10:00 Intermission.

10:20 AGFD 104. Physical stability of solid food products: Development and applications of material science within Nestlé since 30 years. **V. Meunier**

10:50 AGFD 105. Water mobility approach to food product development. **Y. Kou**

11:20 AGFD 106. A decade of work: Developing applications for dynamic moisture sorption curves. **B. Carter**

Section B
Ernest N. Morial Convention Center
Room 217

Withycombe-Charalambous Graduate Student Symposium

K.D. Deibler**,** *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 AGFD 107. Engineered bacteriophage-based electrochemical detection of *Escherichia coli* in food samples. **D. Wang**, J. Chen, T. Hinkley, S.R. Nugen

9:30 AGFD 108. Real-time and *in situ* monitoring and characterization of pesticide residues on and in fresh produce using surface-enhanced Raman spectroscopy. **T. Yang**, L. He

9:55 AGFD 109. Identification of *Bifidobacterium pseudocatenulatum* D2 as a probiotic with anti-inflammatory and anti-cancer potential. **M. Gu**, C. Pan, Z. Gao, H. Xiao

10:20 Intermission.

10:35 AGFD 110. Conjugated linoleic acid regulates body composition and locomotor activity in sex-dependent manners in *Drosophila melanogaster*. **P.B. Chen**, J. Kim, J.M. Clark, Y. Park

11:00 AGFD 111. Development of innovative techniques for food authentication: The last barrier to prevent food fraud. **Y. Hu**, X. Lu

11:25 AGFD 112. Peptidomic profiling of human milk by mass spectrometry revealed pH-specific milk proteolysis. **J. Gan**, J. German

11:50 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 218

Chemistry of Spirits

K.R. Cadwallader, M. Granvogl, M.C. Qian, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 AGFD 113. Flavor chemistry of spirits: An overview. **M.C. Qian**

9:00 AGFD 114. Factors influencing the key aroma compounds of rum. L. Franitza, L. Nicolotti, **M. Granvogl**, P.H. Schieberle

9:25 AGFD 115. Gin still configuration and its impact on botanical oil distillate profiles in final product. **P.S. Hughes**

9:50 AGFD 116. Sensory and volatile analysis of American whiskeys with different mashbills: Can we discriminate rye and bourbon whiskeys? **J. Lahne**, T. Collins, H. Abdi, H. Heymann

10:15 Intermission.

10:30 AGFD 117. Influence of ethanol on flavor perception in distilled spirits. **K.R. Cadwallader**, C. Ickes

10:55 AGFD 118. Characterization of flavor and odor compounds in blueberry beer by GC-MS: Effects of blueberry and hop addition on chemical composition. **K.M. Papson**, **M.C. Crowe**

11:20 AGFD 119. Shaken not stirred, y'all: A comparison of Texas vodkas, part two. **G.R. Shelton**, M. Montoya, S.B. Bach, D.S. Mason

11:45 Concluding Remarks.

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, PRES‡ and MPPG‡

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 216

Water in Foods Symposium in honor of Louise Slade & Harry Levine

Water Structure

J.W. Finley, Y. Roos, *Organizers*
L.J. Mauer, V. Meunier, *Presiding*

1:00 AGFD 120. Sugar stereochemistry effects on water structure and on protein stability: The templating concept. **Y. Livney**, R. Edelman, I. Kusner, R. Kisiliak, S. Srebnik

1:30 AGFD 121. Multiple solvent-slaved dynamic processes in human serum albumin monitored by phosphorescence spectroscopy. A. Draganski, J.M. Friedman, **R.D. Ludescher**

2:00 AGFD 122. Analysis of the frozen state of Sephadex G25 gel by using X-ray CT and XRD. **N. Murase**, Y. Uetake, K. Irie, Y. Ueno, T. Hirauchi, T. Kawahara, M. Hirai

2:30 AGFD 123. Local and mesoscopic-scale water structure and inhomogeneity: Implications for freezing and stability of amorphous pharmaceuticals. **E. Shalaev**, A. Soper, A. Zeitler, S. Ohtake, C.J. Roberts, M.J. Pikal, K. Wu, B. Zakharov, E. Boldyreva

3:00 Intermission.

3:20 AGFD 124. Interactions between biopolymers, solutes and water as controlling factors of the structuring pathway in food matrices: Material science based guidelines for the design of bakery products with improved nutritional profile. **S. Renzetti**

3:50 AGFD 125. Role of large deformation mechanics and osmocapillarity in water holding and drying of biological tissue. **R. van der Sman**

4:20 AGFD 126. 2D ^{1}H T_1-T_2 NMR investigation of standard and gluten free bread during staling. **E. Vittadini**, E. Curti, P. Littardi, E. Carini

Section B
Ernest N. Morial Convention Center
Room 217

Chemistry of Sex

T.E. Acree, J.W. Finley, S.J. Toth, M.H. Tunick, *Organizers*
K.D. Deibler, A.E. Mitchell, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 127. Mind of sexual chemistry: How foods, fragrances, situations, and people drive the expectation of erotic encounters. A. Gere, D. Radványi, P. Papajorgji, **H. Moskowitz**

1:30 AGFD 128. Fragrance and attraction. **A.P. Narula**

1:55 AGFD 129. Chemistry of chocolate and pleasure. **M.H. Tunick**, J.A. Nasser

2:20 AGFD 130. Wine and sex: Potential effects of odorants on sexuality. **T.E. Acree**, A. Barwich

2:45 AGFD 131. Environmental toxicants: "The elephant in the room" risk factor for male sexual dysfunction. **L.M. Alzweri**, A.L. Burnett, W.J. Hellstrom, S.C. Sikka

3:10 Intermission.

3:25 AGFD 132. Bitterness of active pharmaceutical Ingredients (API): From Advil® (ibuprofen) to Viagra® (sildenafil). **K.D. Deibler**

3:50 AGFD 133. Sex toys, edible underwear, and personal lubricants: Applying food safety principles to sex paraphernalia design. **R. Worobo**

4:15 AGFD 134. Wavelength dispersive x-ray flouresence (WDXRF) for elemental analysis of sexual performance supplements, edible garments, gummies and lubricants. **A.E. Mitchell**, T. Nguyen, G. Williams

Section C
Ernest N. Morial Convention Center
Room 218

Chemistry of Spirits

K.R. Cadwallader, M. Granvogl, M.C. Qian, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 135. Characterization of the key aroma compounds in *Meilanchun* sesame flavor style Baijiu by aroma extract dilution analysis, quantitative measurements, aroma recombination, and omission/addition experiments. **M. Huang**, Q. Li, S. Luo, B. Sun, F. Zheng, J. Sun, X. Sun, H. Li

1:30 AGFD 136. Key flavor compounds in ultra-aged tequila. **A. Aguirre-Flores**, Y.L. Qian, P. Vazquez, M.C. Qian

1:55 AGFD 137. Characterization of key aroma compounds in Gujinggong Chinese Baijiu by gas chromatography–olfactometry, quantitative measurements, and sensory evaluation. **J. Sun**, D. Zhao, D. Shi

2:20 Intermission.

2:35 AGFD 138. Determination of volatile compounds in Chinese *Baijiu-Laobaigan* by comprehensive two-dimensional gas chromatography/high resolution-time of flight mass spectrometry. **Y. Ma**, J. Sun, F. Zheng, H. Li, Y. Zhang, F. Zhang, B. Sun, F. Chen

3:00 AGFD 139. The soul of "Qingke" liquor from Tibet. **Y.L. Qian**, S. Chen, M.C. Qian

3:25 Concluding Remarks.

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, PRES‡ and MPPG‡

Nexus of Food, Energy, & Water: Adapting to Future Challenges
Sponsored by MPPG, Cosponsored by AGFD‡, ENFL‡ and ENVR‡

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Value Added from Agricultural Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

Undergraduate Research Posters

Agricultural and Food Chemistry

Sponsored by CHED, Cosponsored by AGFD and SOCED

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 216

Water in Foods Symposium in honor of Louise Slade & Harry Levine

Water & Stability

J.W. Finley, Y. Roos, *Organizers*
B. Carter, S. Mizrahi, *Presiding*

8:00 AGFD 140. Water of crystallization in pharmaceutical products. **J. Rantanen**

8:30 AGFD 141. Predicting the crystallisation of sugar in dried raisins and honey. **B. Bhandari**, D. Dahal, T. Truong, P. Urrutia, S. Almonacid

9:00 AGFD 142. Role of water in food powders: process/product interactions. **S. Desobry**, P. Schuck

9:30 AGFD 143. Effect of polyols on the stability of dairy proteins in high protein systems. **P. Zhou**

10:00 Intermission.

10:20 AGFD 144. Chemical stability in low and intermediate moisture systems: The role of water activity and glass transition. **L.N. Bell**

10:50 AGFD 145. Water in starch,

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laponite and in its nanocomposite films. G. Ayala Valencia, M. Djabourov, F. Carn, **P. do Amaral Sobral**

11:20 AGFD 146. Applications of probabilistic engineering in food moisture management to meet product quality, safety and shelf-life requirements. **J. Torres**, V. Rodriguez Martinez, G. Velazquez, J. Welti-Chanes

Section B
Ernest N. Morial Convention Center Room 217

Kenneth A. Spencer Award Symposium

Cosponsored by AGRO
E. Hellmuth, *Organizer*
W.H. Yokoyama, *Organizer, Presiding*

8:30 AGFD 147. Modernizing polysaccharide analysis: An LC/MS-based platform for characterizing nature's most difficult biomolecule. **M. Amicucci**, C.B. Lebrilla

9:00 AGFD 148. Impact of milk on the metabolic phenotype of the developing neonate. **C. Slupsky**

9:30 AGFD 149. Using genomics and glycomics to investigate bioactive oligosaccharide production in dairy cows. **R.C. Robinson**, N.A. Poulsen, L.B. Larsen, D. Barile

10:00 Intermission.

10:10 AGFD 150. The Kenneth A. Spencer Award. **J.N. Seiber**

10:25 AGFD 151. Recent milk genomics research and the discovery of probiotic carbohydrate constituents. **J. German**

Section C
Ernest N. Morial Convention Center Room 218

Environmental Effects on Gulf Coast Seafoods

E.S. Maung-Douglass, *Organizer*
J.W. Finley, D. Holliday, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 152. Quality and safety of Gulf seafood is some of the finest in the world. **D.L. Holliday**, J.W. Finley, M.A. Tarr

8:30 AGFD 153. Modeling 3D fish movement in the Gulf of Mexico hypoxic zone. **E. LaBone**, D. Justic, K. Rose, L. Wang, H. Huang

8:55 AGFD 154. Petroleum hydrocarbons in coastal environments of the northern Gulf of Mexico after Deepwater Horizon oil spill. **Z. Liu**

9:20 AGFD 155. Ag nutrient use in Illinois: Meeting N & P loss reduction goals by 2025 against all odds. **J. Payne**

9:45 AGFD 156. Distribution of dispersant-related surfactants in the Gulf of Mexico area following the Deepwater Horizon oil spill. **J. Gray**, L.K. Kanagy, C.J. Kanagy, J.W. McCoy, E.T. Furlong

10:10 Intermission.

10:30 AGFD 157. "Farming" seafood following a marine oil spill: Seafood safety and perspectives from harvesters, consumers, and public health scientists. **J. Wickliffe**, B.R. Simon-Friedt, M.J. Wilson, J.L. Howard, E. Frahm, D. Nguyen, D. Gauthe, B. Meyer, D. Pangeni, E.B. Overton

10:55 AGFD 158. Oil spilled in marine systems: Photochemistry and impacts on aquatic organisms. **M.A. Tarr**, X. Cao, P. Zito, D.C. Podgorski, B.H. Harriman, J.M. Suflita, S. King, T.M. Soniat, M.A. Thorne

11:20 AGFD 159. Estimated effects on fish larvae of water column polycyclic aromatic hydrocarbons (PAH) during and after the Deepwater Horizon (Macondo) incident. **T.L. Wade**

11:45 AGFD 160. Health effects associated with dispersant exposure during the Deepwater Horizon oil spill response: Findings from the GuLF STUDY. **L. Engel**, C. McGowan, K. Gam, M. Curry, R. Kwok, M. Lichtveld, A. Miller, M. Stenzel, P. Stewart, D. Sandler

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Sponsored by GEOC, Cosponsored by AGFD, AGRO and ENVR

Biobased Water Purification System Approaches
Sponsored by CELL, Cosponsored by AGFD, CHAS and ENVR

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Food, Water & Energy from Sustainable Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center Room 216

Water in Foods Symposium in honor of Louise Slade & Harry Levine

The Glassy State

J.W. Finley, Y. Roos, *Organizers*
P. Buera, D. Champion, *Presiding*

1:00 AGFD 161. Powder structure and the influence of water from drying to dissolution. **A. Millqvist Fureby**

1:30 AGFD 162. Role of water in encapsulation of food ingredients. **S. Drusch**

2:00 AGFD 163. Thermal properties and molecular mobility of amorphous trehalose-limonene matrices obtained by different glass-forming approaches: Desolvatation vs. solid state. **P. Pittia**, M. Faieta, M. Geppi, F. Panattoni, L. Neri

2:30 Intermission.

2:50 AGFD 164. Evaluation of water sorption and thermal properties of galacto-oligosaccharides, and application in glassy confections. **Y. Vodovotz**

3:20 AGFD 165. Enhanced thermotolerance of probiotic cells during dynamic droplet drying compared to heat treatment. **N. Fu**, X.D. Chen

3:50 Concluding Remarks.

Section B
Ernest N. Morial Convention Center Room 217

Kenneth A. Spencer Award Symposium

Cosponsored by AGRO
E. Hellmuth, *Organizer*
W.H. Yokoyama, *Organizer, Presiding*

1:00 AGFD 166. The evolution of interesterified lipids from curiosity to designer lipids for food and pharma application. **J.W. Finley**

1:30 AGFD 167. Development of an immunoassay for amanitin, a highly toxic mushroom toxin. **C. Bever**, B. Barnych, L.H. Stanker

2:00 AGFD 168. Identification of botulinum neurotoxin serotype A inhibitors using in vitro cell and oral models of intoxication. **L. Cheng**, C. Tam, L.H. Stanker

2:30 AGFD 169. Stability, bioavailability, and detection of abrin. **C. Tam**, L.H. Stanker, L. Cheng

3:00 Intermission.

3:10 AGFD 170. Fiber and polyphenolics that prevent metabolic dysfunction in diet induced animal models. **W.H. Yokoyama**, H. Kim, T. Arvik

3:40 AGFD 171. Bioactive lipid profiles as indicators of exposure. **M.L. Nording**

4:10 AGFD 172. Adsorption behavior of sunflower lecithin at an air-water interface: Role of lysolecithin. **J. Staton**, S.R. Dungan

4:40 AGFD 173. Local equilibrium flavor distributions in short-chain lecithin solutions. **A. Karman**, S.R. Dungan, N. Nitin, S.E. Ebeler

Section C
Ernest N. Morial Convention Center Room 218

Career Trajectories for Ag & Food Chemists: Panel Discussion

B.D. Guthrie, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 AGFD 174. My career as a regulatory scientist at U.S. Food and Drug Administration. **L. Jackson**

1:20 AGFD 175. Career trajectories in agricultural and food chemistry: An academic path. **A.E. Mitchell**

1:30 AGFD 176. My career path as an industrial agriculture and food chemist. **S.J. Toth**

1:40 Panel Discussion.

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Sponsored by GEOC, Cosponsored by AGFD, AGRO and ENVR

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Biomaterials Processing

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center Room 216

General Papers

Pesticides, Herbicides & other Active Natural Chemicals

B.D. Guthrie, *Organizer*
K.D. Deibler, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD 177. Substantial reduction of herbicide application rates using a novel nanostructured pesticide delivery technology. **E. Manek**, R.V. Jones, F. Darvas

8:25 AGFD 178. N-halamine surface functionalization of stainless steel substrates with dual antimicrobial and regenerable character for potential use in the food industry. **B. Demir**, S.D. Worley, R. Broughton, T. Huang, M.J. Bozack

8:45 AGFD 179. Determination of ionic herbicides in beverages and fruit samples using ion chromatography coupled with high resolution accurate mass spectrometry. **T. Christison**, S. Adams, R. Fussel, J. Beck, J. Rohrer

9:05 AGFD 180. Fatty acids profiling as a biomarker of exposure to pesticides. F.H. Abdel-Rhman, D. Adisa, O. Owopetu, P.S. Henry, **S. Jamadar**, K. Anthony, T. Nguyen, B.L. Wilson, M.A. Saleh

9:25 AGFD 181. Fungicide and insecticide dissipation in soil used for sugarcane billet seed treatment. **D. Wayment**, H.J. Ledet, K.A. Torres, C.L. Webber, P.M. White

9:45 AGFD 182. Impact of postharvest ultrasound treatment on physiology and primary metabolic profile of the tomato fruit during storage. **D. Jha**, J. Arul

10:05 Intermission.

10:25 AGFD 183. Withdrawn

10:45 AGFD 184. Essential oil content of the seeds of Wonderful kola, African walnut and Guinea plum and their potentials on hyperlipidemic male Wistar rats. **E.O. Nwaichi**, J. Osuoha, M. Monanu

11:05 AGFD 185. Sampling of 6-methoxybenzoxazolin-2-one (MBOA) from maize seedlings by silicone tube microextraction. **H. Pedersen**, K. Heinrichson, I.S. Fomsgaard

11:25 AGFD 186. Effects of cutting and drying leaves of culinary herbs on contents of bioactive phytochemicals in *Perilla frutescens*. **N. Kagawa**, M. Henzan, H. Iguchi, M. Hanaoka

11:45 AGFD 187. Antibacterial Activity of Ascorbic acid: pH effect, specific action or both? **L. Panda**

Section B
Ernest N. Morial Convention Center Room 217

Up in Smoke: Chemistry of Smoky Odors in Food & the Environment

A. Buettner, B.D. Guthrie, *Organizers*
J. Beauchamp, *Organizer, Presiding*

8:30 Introductory Remarks.

8:50 AGFD 188. Smoky, vanilla

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or clove-like? **A. Buettner**, M. Wagenstaller, K. Lorber

9:20 AGFD 189. Human olfactory receptors: From systematic deorphanization to the identification of olfactory receptors activated by guaiacol and related smoky compounds. **C. Pierre**, M. Philippeau, A. Veithen, S. Huysseune, Y. Quesnel

9:50 AGFD 190. Thermal decomposition of wood derived organic matter under specific industrial process conditions. **M. Backes**, **G.E. Krammer**, B. Voss

10:20 Intermission.

10:35 AGFD 191. Incense materials: How burning lifts our spirits. **A. Buettner**, J. Niebler

11:05 AGFD 192. Changes in aroma and sensory profile of food products smoked in the presence of a zeolite filter. **J.K. Parker**, X. Chua, E. Uwiduhaye, S. Lignou, H.D. Griffiths, D.A. Baines

11:35 AGFD 193. Effect of sugars on vapour partition of volatile compounds of coffee beverages. **P. Pittia**, V. Lonzarich, D. Compagnone, L. Navarini

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Sponsored by CHAS, Cosponsored by AGFD, CHAL and SCHB

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 216

General Papers

Natural Products & Processing Chemistry

B.D. Guthrie, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 194. Lipids of *Silybum marianum* (L.) fruits. **D. Hlangothi**, K. Anthony, M.A. Saleh

1:25 AGFD 195. pH, total acidity, and antioxidant activity of cold brew coffee. **N.Z. Rao**, M. Fuller, M. La Torre

1:45 AGFD 196. Effect of pH and caffeine concentration on the hydrolysis of starch by α-amylase. F. Medina, R.J. Straw, A.N. Shaffer-Doan, **A. Khan**

2:05 AGFD 197. Bioproducts potential of *Cladophora glomerata* Algae. **W. Gao**

2:25 AGFD 198. Different Brazilian cold-pressed oils: Chemical composition and healthy properties. N. Cicero, **R. Tardugno**, A. Albergamo, D.G. Bua, V. Di Stefano, A. Salvo, V. Mangano, A. Rotondo, G. Di Bella, G. Dugo

2:45 AGFD 199. Exposure of mint plants to light emitted diode (LED) lights and their impact on essential oil composition. **T. Nguyen**, M.A. Saleh

3:05 Intermission.

3:25 AGFD 200. Green and effecient extraction of highly crosslinked sorghum protein with preserved backbones. **W. Li**, B. Mu, H. Xu, L. Xu, Y. Yang

3:45 AGFD 201. Chemical profiling of rare South American red nectar. **S. Chakraborty**, J. Jones, M. Phan, N.M. Glagovich, Y. Cai, T. Mione

4:05 AGFD 202. Characterizing germinated brown rice milk beverage processes using green technologies. **J. Beaulieu**, S. Boue, S. Reed, K. Daigle

4:25 AGFD 203. Composition and structural features of condensed tannins from Texas legumes exhibiting methane abatement activity during *in vitro* rumen digestion. H.D. Naumann, R. Sepela, A. Rezaire, A.E. Hagerman, L.A. Reinhardt, J.T. Robe, **W. Zeller**

4:45 AGFD 204. Pigmented tannin by polar chromatography tandem MS for identification of candidate molecular features. **A.L. Waterhouse**, J.R. Cave, C.B. Lebrilla, E.A. Parker

Section B
Ernest N. Morial Convention Center
Room 217

Up in Smoke: Chemistry of Smoky Odors in Food & the Environment

J. Beauchamp, B.D. Guthrie, *Organizers*
A. Buettner, *Organizer, Presiding*

1:00 AGFD 205. Wheat beer aroma: Which molecules are evoking the typical desired clove-like and smoky aroma? **M. Granvogl**, D. Langos, P.H. Schieberle

1:25 AGFD 206. Characterization of smoke produced by the New Zealand native plant species, Manuka. **Y. Zhang**, M. Macalister, G. Eyres, J. Jones, P. Silcock

1:50 AGFD 207. Uptake of smoke derived volatile phenols by grapevines and their impact on wine composition and sensory properties. **R. Ristic**, L. van der Hulst, K. Wilkinson

2:15 AGFD 208. Fumé, flint and fire: Smoky flavors in wine. **M. Herderich**

2:40 Intermission.

2:55 AGFD 209. Rapid determination of "smoky" odorant thresholds in red wine using sniff olfactometry (SO). **T.E. Acree**, D. Perry, M. Gros, A. Vigueras, A.K. Mansfield

3:20 AGFD 210. Withdrawn

3:45 AGFD 211. Rapid quantitation of phenolic compounds in Islay whiskies by direct injection mass spectrometry. **J. Beauchamp**

4:10 AGFD 212. Thin-Film SPME: A novel approach to the analysis of polar flavor molecules in beverages. **K. Thaxton**, J.R. Stuff, J. Whitecavage

4:35 Concluding Remarks.

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Sponsored by CHAS, Cosponsored by AGFD, CHAL and SCHB

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 216

General Papers

Analysis & Methods

B.D. Guthrie, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 AGFD 213. Optimization of reducing sugar-PMP reactions by response surface methodology. **W. Wang**, F. Chen, Y. Wang

8:25 AGFD 214. Animal fat waste and cooking oil waste: A potential source for biodiesel. **M.A. Saleh**

8:45 AGFD 215. Stability of dietary nitrate, phenolic compounds and enhancement of nitric oxide precursor by different vegetable juices blending. **B. Patil**, K.A. Corleto, J. Singh, G.K. Jayaprakasha

9:05 AGFD 216. Physicochemical properties of *Blighia sapida* (ackee) oil. **J.J. Clarke**

9:25 AGFD 217. Chromatographic method validation for cannabis labs: Addressing unique industry challenges. **A. Rigdon**, J. Kowalski, C. Sweeney, J. Cochran, B. Cassidy

9:45 AGFD 218. Starch synthesis in soft white wheat and the biochemical changes induced by sprouting. **Y. He**, M. Tsai, F. Fang, K. Schroeder, A. Lin

10:05 Intermission.

10:25 AGFD 219. Coupling of wet chemistry methods and spectroscopic data for elucidating composition and structure of purified condensed tannins. **W. Zeller**, I. Mueller-Harvey, A.E. Hagerman

10:45 AGFD 220. Omics forecasting: Predictive calculations permit the rapid interpretation of high resolution mass spectral data from complex mixtures. **J.R. Cave**, A.L. Waterhouse

11:25 AGFD 221. Optimizing espresso: Chemical and physical considerations, and a step towards reproducibly tasty coffee. **C.H. Hendon**, W. Lee, J. Foster

11:45 AGFD 222. Determination of organic acids in animal feed using two ion chromatography methods. **J. Hu**, J. Rohrer

Section B
Ernest N. Morial Convention Center
Room 217

Chemistry & Applications for Cotton

S. Chang, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 AGFD 223. Effect of pre-heating on the thermal decomposition kinetics of cotton. **S. Nam**, B.D. Condon

9:05 AGFD 224. Innovative technologies development for anti-flammable cotton fabrics at USDA. **S. Chang**, B.D. Condon, J. Smith

9:35 AGFD 225. Correlating metals present in soil and cotton fiber. **C.A. Fortier**

10:05 Intermission.

10:25 AGFD 226. Cytotoxicity and gene expression regulation of minor components from cottonseeds in mouse RAW macrophages. **H. Cao**, K. Sethumadhavan

10:55 AGFD 227. Examination of cotton fiber bundle properties using an infrared focal plane array detector. **M. Santiago**, T. Von Hoven, D. Hinchliffe

THURSDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 216

General Papers

B.D. Guthrie, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD 228. ANOVA for unbalanced data: Using spreadsheets to evaluate sums of squares and comparisons of means. **T. Klasson**

1:25 AGFD 229. Withdrawn

1:45 AGFD 230. Interactions between polysaccharides and flavonoids: Potential contribution to microstructure in wine. **T. Goulette**, E.A. Decker, H. Xiao, H. Chong, M.T. Cleary

2:05 AGFD 231. Determination of flavonoids, alkaloids and saponins in *Solanum scabrum* berries using LC/UV/MS. **B. Yuan**, D. Byrnes, J. Simon, Q. Wu

2:25 AGFD 232. The quantification of the food water and energy nexus and cost analysis associated with resource consumption and reduction within a milk processing facility. **C. Adams**

2:45 Intermission.

3:05 AGFD 233. Preparation and characterization of quercetin-loaded electrospun fiber mat and its colon-specific release property. **P. Wen**, M. Zong, H. Wu

3:25 AGFD 234. Withdrawn

3:45 AGFD 235. Storage conditions affect the untargeted chemical profile and bioactivity of black raspberry nectar intended for use in clinical trials. **M.D. Teegarden**, T.J. Knobloch, C.M. Weghorst, J. Cooperstone, D.G. Peterson

4:05 AGFD 236. Inhibitory effect of aqueous extract of the potato peel waste on starch digestive enzymes. **C. Chen**, S. McGeehan, M. Thornton, A. Lin

AGRO

Division of Agrochemicals

J. Eble, *Program Chair*

SUNDAY MORNING

Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes
Sponsored by GEOC, Cosponsored by AGRO and ENVR

SUNDAY AFTERNOON

Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes
Sponsored by GEOC, Cosponsored by AGRO and ENVR

TUESDAY MORNING

‡*Cooperative Cosponsorship*

Kenneth A. Spencer Award Symposium
Sponsored by AGFD, Cosponsored by AGRO

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Sponsored by GEOC, Cosponsored by AGFD, AGRO and ENVR

TUESDAY AFTERNOON

Kenneth A. Spencer Award Symposium
Sponsored by AGFD, Cosponsored by AGRO

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Sponsored by GEOC, Cosponsored by AGFD, AGRO and ENVR

WEDNESDAY EVENING

Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes
Sponsored by GEOC, Cosponsored by AGRO and ENVR

ANYL

Division of Analytical Chemistry

L. Baker and M. Bush, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Failed Brilliance in Nanocellulose Science & Technology (see *CELL*, Sun)

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries (see *CELL*, Sun, Mon)

Advances in Bacterial (Nano) Cellulose Research (see *CELL*, Thu)

Inaugural Joint Symposium of the Separation Science Subdivisions (see *I&EC*, Wed)

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium (see *PROF*, Sun, Mon)

Polymer Colloids: Synthesis, Analysis, Modeling & Applications (see *POLY*, Sun, Mon, Tue, Wed)

SOCIAL EVENTS:

ANYL Reception, 5:00 PM: Tue

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 228

Challenges in Determining Arsenic Compounds in Rice
Cosponsored by MPPG‡
P.J. Gray, J.F. Tyson, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 ANYL 1. Rice consumption and adverse health outcomes: What do we know? **M. Karagas**

9:20 ANYL 2. Chemical analyses in support of studies of the health implications of rice consumption. **B.P. Jackson**, M. Karagas, T. Punshon, K.L. Cottingham

9:50 Intermission.

10:10 ANYL 3. Current and future FDA arsenic speciation methods. **P.J. Gray**

10:40 ANYL 4. Determination of arsenic in baby cereal. **J. Nelson**

11:10 ANYL 5. Lessons learned in arsenic speciation: The good, the bad, and the painful. **M. Kelinske**

11:40 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 230

Microfluidic Electrochemical Bioanalysis

M.H. Shamsi, *Organizer*
M. Shamsi, *Presiding*

8:30 Introductory Remarks.

8:35 ANYL 6. Low-cost bioassay developement for resource-constrained settings. **W. Asghar**, **M. Sher**

9:05 ANYL 7. 3D-printed integrated microfluidic devices for biomolecular assays. **A. Woolley**, M. Beauchamp, E.K. Parker, A.V. Nielsen, H. Almughamsi, H. Gong, G.P. Nordin

9:40 ANYL 8. Development of electrochemical multiplex 3-D sensors. **Z. She**, K. Topping, D. Kelly, H. Kraatz

10:05 Intermission.

10:20 ANYL 9. Electrochemical paper-based analytical devices for clinical and environmental diagnostics. **C. Henry**, B. Geiss, J. Volckens

10:55 ANYL 10. Electrochemical, aptamer-based sensing supports real-time, closed-loop control of plasma drug levels directly in the body of live animals. **N. Arroyo**

11:20 ANYL 11. Electrochemical study of hexanucleotide repeat expansion linked with neurodegenerative diseases. **M. Shamsi**

Section C
Ernest N. Morial Convention Center
Room 229

Ultrafast Spectroscopy Meets Chemistry, Materials & Biology

Novel Approaches

K.W. Huang, I.V. Rubtsov, J. Zheng, *Organizers, Presiding*

9:00 Introductory Remarks.

9:10 ANYL 12. Ultrafast shock compression spectroscopy meets chemistry, materials and biology. **D.D. Dlott**

9:45 ANYL 13. Ultrafast single-molecule electrical detection. **X. Guo**

10:20 Discussion.
10:30 Intermission.

10:45 ANYL 14. Monitoring nonadiabatic dynamics and conical intersections by nonlinear broadband X-ray spectroscopy. **S. Mukamel**

11:20 ANYL 15. Quantum coherence in ultrafast molecular processes: *ab initio* simulations including dephasing. **E. Coccia**, S. Corni

Section D
Ernest N. Morial Convention Center
Room 227

Wearable & Implantable Sensors
Cosponsored by MPPG‡
M.A. Daniele, L. Deravi, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ANYL 16. Persistent drought monitoring using a microfluidic-printed electro-mechanical sensor of stomata *in planta*. **V. Koman**, T. Lew, S. Kwak, M. Wong, J. Giraldo, M. Strano

8:50 ANYL 17. Microfluidic encapsulation of nanomaterials for implantable biosensors. **W. Zhang**, X. Xie, A. Abbaspourrad, D.A. Weitz, D.G. Anderson

9:05 ANYL 18. Chemically tuned thin-film and nanofluidic sensors for single-molecule and particle sensing. **J.R. Dwyer**, B.I. Karawdeniya, Y.D. Bandara, J.W. Nichols

9:35 ANYL 19. Design and manufacture of three-dimensional paper-based microfluidic devices. **C. Mace**, S. Fernandes, D. Wilson, N. DeChiara, J. Brooks

10:05 ANYL 20. Interfacing and reverse engineering of live tissue operation in hydrogel microfluidic devices for wearable sensors. **O.D. Velev**, T. Shay, M.D. Dickey

10:35 Intermission.

10:50 ANYL 21. Nanocomposite microneedles for extraction, sampling, and separation of dermal interstitial fluid. E. Marrow, A. Kiran, H. Nissan, A.T. Young, **M.A. Daniele**

11:20 ANYL 22. Microneedles to monitor health and human performance. **R. Polsky**

11:50 ANYL 23. Withdrawn

Section E
Ernest N. Morial Convention Center
Room 226

Open Resources for Automated Structure Verification & Elucidation

E. Schymanski, A.J. Williams, *Organizers, Presiding*

8:30 ANYL 24. Overview of open resources to support automated structure verification and elucidation. **A.J. Williams**, E. Schymanski

8:55 ANYL 25. Using open resources for structure dereplication. **D. Argyropoulos**, S. Golotvin, R. Pol, J. DiMartino, A. Moser

9:20 ANYL 26. Fast search chemical structure in 90 million publicly available known compounds by NMR and MS. T. Churanova, **K. Blinov**

9:45 ANYL 27. Improved structure elucidation and verification results with optimized NMR data acquisition methods and strategies. **C. Anklin**, N. Kruse

10:10 Intermission.

10:35 ANYL 28. Using the US EPA's CompTox Chemistry Dashboard for structure identification and non-targeted analyses. **A.J. Williams**, A. McEachran, S. Newton, K. Isaacs, K. Phillips, N. Baker, C. Grulke, J. Sobus

11:00 ANYL 29. Curating "suspect lists" for international non-target screening efforts. **E. Schymanski**, R. Aalizadeh, N.S. Thomaidis, J. Hollender, J. Slobodnik, A.J. Williams

11:25 ANYL 30. Open source software platform for mass spectrometry based non-target screening in the environment. **R. Helmus**, V. Albergamo, O. Brock, J. Parsons, P. de Voogt

11:50 ANYL 31. *mz*CLOUD: A spectral tree library for the Identification of "unknown unknowns". **R. Mistrik**

12:15 ANYL 32. Automated structure annotation and curation for MassBank: Potential and pitfalls. **E. Schymanski**, M. Stravs, T. Schulze, A.J. Williams

12:40 Discussion.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

Failed Brilliance in Nanocellulose Science & Technology
Sponsored by CELL, Cosponsored by ANYL

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 228

Challenges in Determining Arsenic Compounds in Rice
Cosponsored by MPPG‡
P.J. Gray, J.F. Tyson, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 ANYL 33. Performance comparison between extraction methods to support arsenic speciation analyses in rice and rice products. **R. Gerads**

2:10 ANYL 34. Determination of inorganic arsenic in rice by hydride generation, Peltier-effect cryogenic trapping and atomic fluorescence spectrometry. **G. Chen**, B. Lai, M. Xuefei, T. Chen, M. Chen

2:40 Intermission.

3:00 ANYL 35. Methods based on field test kits. **J.F. Tyson**, N. Fragola, C. Zhang

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3:30 ANYL 36. A scalable field test method to speciate arsenic in rice for less than $2 per sample. **P.J. Gray**

4:00 Panel Discussion.
5:20 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 230

Plant Omics
Cosponsored by CELL and MPPG‡
L.M. Hicks, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ANYL 37. Temporal-omics, incorporating time into high-throughput plant-omics. **C. Doherty**, J. Desai, D. Grinevich

2:00 ANYL 38. Regulation of chromatin structure by a clade of plant-specfic, circadian clock associated kinases. M. Wilson, S. Tzeng, X. Jiang, L. Ji, J. Choi, J. Butler, R. Schmitz, B.S. Evans, **D.A. Nusinow**

2:25 ANYL 39. Dissecting kinase signaling pathways in plant stress response. C. Hsu, P. Wang, J. Zhu, **W.A. Tao**

2:50 ANYL 40. Integrative network-centric approaches identify signaling networks associated with plant resistance to pathogens. **S.C. Popescu**, G. Popescu, E.K. Brauer, D. Singh

3:15 Intermission.

3:25 ANYL 41. Complexities of N-terminal protein maturation and stability in chloroplasts. **K. van Wijk**

3:50 ANYL 42. Heterotrimeric G-proteins as regulators of cellular redox status in plants. **S. Pandey**, E. McConnell, A. Vijayakumar, S. Roy Choudhury, L.M. Hicks

4:15 ANYL 43. Hyphenated metabolomics of stomatal guard cell responses to CO_2 in the changing climate. **S. Chen**

4:40 ANYL 44. Characterization of metabolic variability in red wines using a highly selective non-targeted acquisition approach. **L.G. Mullin**, R.S. Plumb

5:05 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 229

Ultrafast Spectroscopy Meets Chemistry, Materials & Biology

Reaction Dynamics

K.W. Huang, I.V. Rubtsov, J. Zheng, *Organizers, Presiding*

1:30 ANYL 45. Controlling polyatomic dissociation dynamics using the radical cation launch state. **R.J. Levis**

2:05 ANYL 46. Toward a theory of infra-red perturbed electron transfer reactions. **D.N. Beratan**

2:40 ANYL 47. Dynamics and mechanism of UVR8 photoreceptor. **D. Zhong**

3:15 Intermission.

3:25 ANYL 48. Ultrafast primary process of photo-responsive proteins revealed by femtosecond Raman spectroscopy. **T. Tahara**

4:00 ANYL 49. Exploring dissociation dynamics in families of methylphosphonates and nitrotoluenes with femtosecond pump-probe measurements. **K. Tibbetts**

4:35 ANYL 50. Comparison of photoinduced ultrafast dynamics of semiconducting rare-earth and transition-metal chalcogenides. **D. Yang**, X. He, N. Punpongjareorn

Section D
Ernest N. Morial Convention Center
Room 227

Wearable & Implantable Sensors
Cosponsored by MPPG‡
M.A. Daniele, L. Deravi, *Organizers, Presiding*

1:30 ANYL 51. Flexible electronics and oral biosensing. **D. Schwartz**, R. Street, B. Krusor, P. Mei, A. Pierre, A. Karajic, M. Stambaugh, J. Wang, P. Mercier

2:00 ANYL 52. Liquid metals for wearable sensors. **M.D. Dickey**, T. Shay, O.D. Velev

2:30 ANYL 53. Wearable sensors utilizing nanofiber technology. H. Gao, D. Asheghali, Y. Kim, S. Sharma, **S. Minko**

3:00 ANYL 54. Light-scattering nanostructures enhance visible color in bio-derived textiles. **L. Deravi**

3:30 Intermission.

3:45 ANYL 55. Body powered wearable sensors for personal health and personal environmental monitoring. **V. Misra**

4:15 ANYL 56. Wearable sweat sensors. **A. Javey**

4:45 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 226

Active Learning in the Undergraduate Analytical Chemistry Curriculum

A.G. Cavinato, P. Doolittle, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ANYL 57. Studio classroom as a student-centered active learning environment in undergraduate chemistry courses. **C. Akbay**, D.E. Autrey, E. Oshita

1:55 ANYL 58. Active learning approach in teaching statistics for analytical chemistry laboratory. **N.N. Mateeva**, I. Ivanov

2:15 ANYL 59. What's the buzz!? Undergraduate investigations of caffeine and other chemicals using analytical techniques. **J.R. Kraly**

2:35 ANYL 60. Real-world ready environmental monitoring in the Yellow Water River watershed by intrumental analysis students. **P.D. Voegel**

2:55 Intermission.

3:10 ANYL 61. A research-based experience for the undergraduate analytical chemistry laboratory. **C.D. Walsh**

3:30 ANYL 62. Determining the concentration and speciation of iron in beer samples using a cloud point extraction technique for sample preparation coupled with absorbance and emission spectroscopy. **P. Doolittle**, L. Khalafi, J.C. Wright

3:50 ANYL 63. Nanoparticles for sensor development: An active learning experiment for the analytical chemistry laboratory. **A.G. Cavinato**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall E

Analytical Chemistry in the Developing World

C.J. Brady, A. Cooper, M. Lieberman, *Organizers*

7:00–9:00

ANYL 64. Fighting low quality pharmaceuticals through the development and optimization of an affordable paper-medium antibiotic assay. **A. Cooper**, M. Lieberman

ANYL 65. Determining milkfat content on a paper-based analytical device. **V. Henry de Frahan**, J.L. Luther, M. Lieberman

ANYL 66. Keep the lead away: Understanding the problem of lead in St. Joseph County, Indiana. **M. Dowd**, M. Lieberman

ANYL 67. Algal biodiesel conversion and characterization for use as decentralized electrical energy. **M. Tetrick**, A. Mechtenberg, S. Wietstock, M. Musaazi, J. Makanda

ANYL 68. Synthesis of novel oxazoline compounds for use as insecticides and the evaluation for mosquitocidal and larvalcidal activity. **A.M. Nemeth**, B. Melancon, M.A. McDowell

ANYL 69. In-membrane exploitation of antigen/antibody interaction for selective purification and quantification of therapeutic monoclonal antibodies. **C. Stanton**, J. Berwanger, M. Bruening

ANYL 70. Development of a microfluidic tunable attribute precision screening (TAPS) antimicrobial system for characterization of bacterial stress. **C.J. Brady**, D. Chen, A. Dimkovikj, J. Shuttleworth, J. Shrout, A. Timperman

ANYL 71. Development of a phosphate biosensor using the optical density and pressure of growing yeast. **K. Dwyer**

ANYL 72. Development of a portable biosensor for detection of hormones in technology limited settings. **R. Miller**, A.A. Weaver, M. Lieberman, H.V. Goodson

ANYL 73. Paper test card for detection of adulterated milk (MilkPAD). **J.L. Luther**, V. Henry de Frahan, M. Lieberman

ANYL 74. Validation by LC-MS of paper analytical devices of azithromycin and amoxicillin/clavulanate. **K. Favazzo**, T.L. Barstis, C.J. Dunlap, **S. Lawler**

ANYL 75. Validation by LC-MS of paper analytical devices of suspect nepali omeprazole. **K. Dvorak**, **E. Innis**, K. Favazzo, S. Lawler, T.L. Barstis, C.J. Dunlap

ANYL 76. Using ICP-OES to quantify arsenic levels of leachate samples collected in Nepal. **C. Weston**, R. Shakya, **G. McNamee**, T.L. Barstis, B. Giri

ANYL 77. HPLC verification of paper analytical devices to screen for low-quality albendazole. **H. DiLallo**, T.L. Barstis

ANYL 78. Quantitation of heavy metal concentrations in Nepali leachate samples via ICP-OES analysis. **C. Breakfield**, **A. Shadid**, T.L. Barstis, B. Giri, R. Shakya

ANYL 79. Measuring mercury contamination in Nepali leachate samples. **E. Najacht**, R. Shakya, B. Giri, T.L. Barstis

ANYL 80. Determination of lead(II) levels in raw chicken samples using UV-vis spectrophotometry. **S. Wilson**

ANYL 81. Improving isoelectric focusing on microfluidic devices. **A.A. Anye**, C.T. Culbertson, S.H. Bossmann, K. Sellens

ANYL 82. Screening of biologically important small molecules and transition metal ions by label assisted laser desorption/Ionization mass spectrometry. **A. Mandal**

ANYL 83. Removal of Cu^{2+} and Pb^{2+} from aqueous solution using $K_2Mn_4O_5$ nanomaterial. **B.V. Gonzales**, S.S. Huerta, S. Balboa, J.A. Perez, E. Guevara, J.M. Cantu, C. Valdes, J. Parsons

ANYL 84. Protein-phospholipids conjugates for the design of urea reactive membranes for applications in water purification. **L.N. Santiago-Martoral**, E. Nicolau

ANYL 85. Development of solvent responsive cellulose-block copolymer membranes for the adsorption of emerging organic contaminants. **J. Herrera**, D. Ramos, T. Turley, M. Betancourt, E. Nicolau

ANYL 86. Withdrawn

ANYL 87. Comparing gas chromatography mass spectrometry and infrared spectroscopy methods to identify different polymers. **A. Rubino**

ANYL 88. Microdialysis sampling of

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quorum sensing during biofilm formation. **A.A. Diaz**, R. Liyanage, J.O. Lay, J.A. Stenken

ANYL 89. Insights into structures of compounds in biochar from fast pyrolysis. **Y. Jiang**, D. Ding, A. Talpade, H. Luo, M.M. Abu-Omar, H.I. Kenttamaa

Section A
Ernest N. Morial Convention Center
Hall E

Analytical Division Poster Session

L.A. Baker, *Organizer*

7:00–9:00

ANYL 90. Systematic study of volatile organic compounds released from plastic films using TD-GC/MS and ESI/MS analytical techniques. **L. Huang**, C. Shogbon

ANYL 91. Evaluation of acid vs. base hydrolysis in UPLC-MS/MS analysis of urinary aromatic diamines. **A. Patel**, B. Bowman, D. Bhandari, B. Blount, V. De Jesús

ANYL 92. Artemia as an indicator for stress in saltwater lakes. **M. Morgan**

ANYL 93. Pharmacokinetics of the stereoisomers of VX in guinea pigs following intravenous exposure. **J.M. McGuire**, L.K. Wright, R.L. Kristovich, M.W. Busch

ANYL 94. Withdrawn

ANYL 95. Identification of new classes of thrombin-binding aptamers by microbeads-assisted capillary electrophoresis (MACE) SELEX. **K. Wakui**, T. Yoshitomi, M. Tsuchida, S. Saito, M. Shibukawa, H. Furusho, K. Yoshimoto

ANYL 96. Identification of novel antimicrobial peptides from *Bacillus subtilis* and *Allium sativum* using PepSAVI-MS. **M. Cooke**, N. Parsley, C.L. Kirkpatrick, L. Hicks

ANYL 97. Voltammetric and preliminary computational study of 3-aryl-quinoxaline-2-carbonitrile 1,4-di-N-oxidide derivatives with anti-tumor properties. E.M. Miller, Q. Xia, M.E. Cella, A. Nenninger, M.N. Mruzik, K.A. Brillos-Monia, Y. Hu, R. Sheng, **C. Ragain**, P.W. Crawford

ANYL 98. Microwave spectroscopy of ultracold molecular plasma. **F. Banic Viana Martins**, J.S. Keller, E.R. Grant

ANYL 99. Rapid enrichment and mechanical stimulation of mesenchymal stem cells using dielectrophoresis devices. **J. Yoshioka**, Y. Ohsugi, T. Yoshitomi, T. Yasukawa, N. Sasaki, K. Yoshimoto

ANYL 100. Investigation of isolated particles of lithium ion battery materials using scanning micropipette contact method. **M. Dayeh**

ANYL 101. Withdrawn

ANYL 102. MALDI imaging and laser ablation sampling for analysis of fungicides in produce. **I. Pereira da Silva**, B. Banstola, K. Wang, B.G. Vaz, F. Donnarumma, K.K. Murray

ANYL 103. LC-MS/MS detects urobilinoids from feces in fly guts. **C. Skaggs**, N.E. Manicke, C. Owings, C. Picard

ANYL 104. Plasmonic cross-reactive sensors for biomarker signature profiling. **J.L. Chavez**, J.N. Yoho, B. Geier, C. Grigsby, J.A. Hagen, N. Kelley-Loughnane

ANYL 105. "Signal-on" electrochemical DNA sensors fabricated on electrostatically assisted surface assembly of gold nanostars. **L.A. Mayorga**, K.N. Hipp, Y. Wu, R.Y. Lai

ANYL 106. Monitoring on styrene oligomer derived from debris polystyrene surround Japan and its diffusion to open ocean. K. Amemiya, M. Okada, K. Sumi, M. Ochiai, **K. Koizumi**, H. Sato, K. Takatama, K. Yamada, **K. Saido**, T. Hiaki

ANYL 107. Detection of aromatic amines in human urine: An automated Hamilton STAR/GC/MS/MS method. **S. Mazumder**, R.A. Ahamed, E. McGahee, L. Wang, T.H. Seyler

ANYL 108. The discovery of a racemic compound of pioglitazone hydrochloride that is more stable than the commercial conglomerate. **C. Zhang**

ANYL 109. Comprehensive evaluation of a sub-2 micron chiral stationary phase: Characterization, applications and ultrafast analyses. **M.J. Wilcox**, O. Ismail, F. Gasparrini, G. Mazzoccanti, C. Villani, S. Anderson, A. Cavazzini, M. Catani

ANYL 110. Patchable self-operated ion channel-based mechanoreceptor sensor for health monitoring. **K. Chun**, Y. Son, C. Han

ANYL 111. Fluorescence properties of acriflavine-based GUMBOS and nanoGUMBOS. **B. Manuel**, K.M. Lopez, R.L. Perez, I.M. Warner

ANYL 112. Development of an infrared laser ablation microsampling system. **C. Dong**, F. Donnarumma, K. Wang, C. Szot, K.K. Murray

ANYL 113. Improving relative recovery of cytokines using cibacron blue. **T. Snider**, J.A. Stenken

ANYL 114. Selective sensing of anions with a dinuclear metal complex in water. **A. Hossain**, M. Rhaman, A. Alamgir, D.R. Powell

ANYL 115. Fluorescent sensing and imaging of nicotinamide adenine dinucleotide phosphate in cancer cells. **S. Bae**, S. Shin

ANYL 116. Surface assisted laser desorption ionization mass spectrometry (SALDI-MS) signal enhancement as a function of nanoparticle size/surface area. **J.R. Yount**, **M. Lapak**, S. Ward, J. Schweig, J. Taylor, C. Woolfolk, A. Olaitan, K.S. Molek

ANYL 117. Quick and sensitive UPLC-ESI-MS/MS method for simultaneous quantification of sofosbuvir and its metabolite, GS-331007, in human plasma. **M. Semreen**, H. Alniss, M. Mousa, H. Aboul-Enein

ANYL 118. Development and validation of a stability-indicating UPLC method for naloxone intranasal formulations. **H. Hsu**, M. Al-Ghabeish, C. Abraham, V. Pavuluri, S. Naraharisetti, M. Ashraf, Y. Yang

ANYL 119. Arsenic in infant rice cereals. **J. Ysseldyke**

ANYL 120. Fabrication and evaluation of metal-organic framework/polymer thin film gas sensors. **J. Shankwitz**, G. Szulczewski, A. Hauser

ANYL 121. Chemical features influencing the fingerprinting of polycarboxylates. **F. Lozada**, M. Bonizzoni

ANYL 122. Preparation of immobilized chiral stationary phases based on helical poly(phenylacetylene) derivatives and their applications in enantioseparation by HPLC. **Y. Zhou**, C. Zhang, Q. Geng, L. Liu, H. Dong, T. Satoh, Y. Okamoto

ANYL 123. Development of hollow fiber liquid phase micro-extraction and ultra high performance liquid chromatography-electrospray ionization-mass spectrometry method for trace analysis of 3-methyl-1,2,3-butanetricarboxylic acid in atmospheric aerosols. **H. Abdul-Azeem**, S. Essén, K.E. Stenström, E. Swietlicki, M. Sandahl

ANYL 124. Levoglucosan as a tracer for early detection of smouldering fire. D. Madsen, **H. Abdul-Azeem**, M. Sandahl, B. Husted

ANYL 125. Quantification of trace elements in oil and gas produced waters via ICP-OES versus ICP-MS: Can high tolerance for salinity overcome lower sensitivity? A.M. Jubb, J. McKinley, M. Engle, **C. Danforth**, D. Mueller

ANYL 126. Detection of designer drugs from plasma via paper spray mass spectrometry. **G. Ren**, N.E. Manicke

ANYL 127. Identifying impurities in TBAF. **A. Andreen**, I.A. Brettell-Adams, P.A. Rupar

ANYL 128. Determination of mono-, di-, and trisulfonated quinophthalones in the color additive D&C Yellow No. 10 (Quinoline Yellow) using high-performance liquid chromatography. A. Weisz, **I.C. James**

ANYL 129. Investigation of the sequential flow analysis and the use of chemical reductants for the determination of nitrate in sea water and salt water aquaria. **P.J. Iles**, R. Kochambilli, D. Robison, S. Biehn, C. Woolston, L. Hannibal, L.D. Giddings, R.V. Valcarce, N.R. Bastian, M. Alvarez, R. Holcomb

ANYL 130. Development of an in-field seawater back extraction and HPLC-fluorescence detection of thiocyanate to combat illegal cyanide fishing. **H. Eberlin**, K. Letson, S.K. O'Shea

ANYL 131. Reverse micelles with different functional group pK_as and their application for the detection of acidic peptides. **B. Zhao**, S. Thayumanavan, R.W. Vachet

ANYL 132. Guided inquiry lab research project. **S. Jain**

ANYL 133. Electrochemically synthesized molecularly imprinted polyaniline nanostructure: A recognition matrix for biotinylated targets. **S. Mandal**, S. Suriyanarayanan, I.A. Nicholls, K. Ramanujam

ANYL 134. Development of a paper analytical device for the detection of illicit drugs. **T. Cleary**, M. Lieberman

ANYL 135. Effect of temperature and energy per atom (E/n) in Ar gas cluster ion beam (GCIB, Ar_n^+) on depth profile of organic thin film. **S. Hung**, J. Shyue

ANYL 136. Glyphosate concentrations in river and stream water as a function of rain runoff. **J. Snider**, R.C. Dudek

ANYL 137. Possible functions of transition metal complexes in the catalytic hydrolysis of phosphate esters. **U. Okeke**, R. Butcher, Y. Gultneh

ANYL 138. Photoinduced electron transfer processes of vinylbenzonitrile substituted pyrene: Generation of long-lived charged states. **A. Bhattacharyya**, P. Malakar, P. Edamana

ANYL 139. Filtered Available Phosphate by FIA: Conditions for lower detection limits. **P.J. Iles**, R. Kochambilli, j. Onyeagba, L.D. Giddings, R.V. Valcarce, N.R. Bastian, M. Alvarez, R. Holcomb

ANYL 140. Analysis of fluoride by FIA in dental products. **P.J. Iles**, R. Kochambilli, S. Moore, l. Lester, M. Roberts, L.D. Giddings, R.V. Valcarce, N.R. Bastian, M. Alvarez, R. Holcomb

ANYL 141. Infrared laser ablation of tissue for localized genomics analysis. **K. Wang**, C. Dong, F. Donnarumma, S.W. Herke, K.K. Murray

ANYL 142. Size-dependent oxidation behavior of gold nanoparticles coated with alkanethiol self-assembled monolayers (SAMs). **B.P. Mainali**, F.P. Zamborini

ANYL 143. Adapting a field-deployable mass spectrometer for continuous measurements of helium. **K. Chan**, R. Stanley

ANYL 144. Tip-enhanced laser ablation capture for single cell genomics. **F. Cao**, F. Donnarumma, K.K. Murray

ANYL 145. Determination of biological aminothiols by high performance liquid chromatography coupled with post-column reaction and indirect fluorescence detection. **L. Mikaliunaite**, D.B. Green

ANYL 146. Nanoliter deposition for single cell analysis by MALDI mass spectrometry. **R. Lawal**, F. Cao, F. Donnarumma, **J. Decombe**, R. Duran, K.K. Murray

ANYL 147. Monitoring of lithium enolate formation and quantitation of E vs. Z stereoisomers of a tetrasubstituted vinyl tosylate using inline ReactIR. **F. St-Jean**

ANYL 148. Surface-assisted laser desorption/ionization of small organic molecules using non-functionalized transition metal oxide nanoparticles. **S. Ward**, **J. Schwieg**, M. Lapak, B.A. Zanca, L.F. Barnes, A. McCoy, J.R. Yount, A. Olaitan, K.S. Molek

ANYL 149. Rapid SPE in field HPLC detection of complexed thiocyanate by aqueous soluble metalloporphyrins from saline waters. **K. Letson**, S.K. O'Shea, H. Eberlin

ANYL 150. Top down analysis of on the

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fly hydrogen deuterium exchange of native protein ions. **N. Sanguantrakun**, C. Chanthamontri, M.L. Gross

ANYL 151. Withdrawn

ANYL 152. Preparation of flexible and transparent conductive electrodes using recyclable plastics. **W.C. Sanders**, P.J. Iles, R.V. Valcarce, J. Calara, G. Johnson, A.C. Lines, C. Page, D. Young, M. Vanweerd, G. Hauschild, J. Tigner, W. Hansen, K. Bussard

ANYL 153. Competitive energy transfer and electron transfer in non covalent fullerene dyad. **S. Dutta**, D. Priyadersini, A. Patnaik

ANYL 154. Compact pulsed xenon fluorescence analyzer for simultaneous detection of nanomolar concentrations of nitrite, nitrate, and ammonium in seawater. **R. Masserini**, S.A. Hendrix, K.A. Fanning

ANYL 155. Withdrawn

ANYL 156. Research on the volatile compounds in Gujinggong Baijiu. **H.H. Li**

ANYL 157. Underlying mechanism of freezing-induced aggregation of gold nanoparticles. **K. Hoyt**, A. Marino, J. Heo

ANYL 158. Towards the creation of turn-on fluorescent Schiff base probes for hydrogen sulfide detection. **M. Conte**, A.A. Abd-Elaal, A. Kirtland, Y.I. Lee

ANYL 159. Multi-responsive hydrogel sensors for transition metal ions via Hofmeister series principles. **C. Price**, J. Carroll, T. Lasseter Clare

ANYL 160. Determining the half-life of thiocynate in *amphiprion ocellaris* plasma upon potassium cyanide exposure. **H. Nolte**, J. Brown, N.E. Breen, A. Rhyne

ANYL 161. Investigation of the reusability of affinity surfaces for cell capture and analysis. **R.D. Reif**, E. Hurwitz

ANYL 162. Microfluidic platforms for analyzing the effect of biomimetic templates on calcium phosphate mineralization. **J. Miech**, A.E. Gerdon

ANYL 163. Cobalt protoporphyrin IX nanoparticles provide signal amplification in anodic stripping voltammetry for protein biomarker detection. **R.G. Tzepos**, A.E. Gerdon

ANYL 164. Unmanned aircraft as a tool for localized sampling of carbonaceous air particulate matter. **T.C. Berg**, A. Kubatova, B. Nespor, D. Delene, A. Kubat, J. Moe

ANYL 165. Comparing Pt and carbon as an electrocatalyst support material for dicyanoferriprotoporphyrin in H_2S detection. **J.A. Bennett**, H. Pharathikoune, Y. Qian, S. Simpson, D. Miller, E. Zurek

ANYL 166. Analysis of inks using capillary electrophoresis and direct analysis mass spectrometry techniques. C.L. Copper, **T. Erbach**, **M. McDonough**, N. Drury, M. Moini

ANYL 167. Algae-biotemplated water-splitting nanocatalysts for efficient oxygen evolution reaction. **D. Nde**, W. Zhao

ANYL 168. Analysis of nicotine in clay samples by solvent extraction and gas chromatography mass spectrometry. **J. Ustick**, C. Chuang, D.S. Muesse, J. Russ

ANYL 169. Electrochemical immunosensor for simultaneous determination of IL-6 and IL-22 in serum using nanostructured electrode array coupled to PEG-multilabeled magnetic particle and a microfluidic device. **B.S. Munge**, S. Nedder, M. Boisclair, V. Trudel

ANYL 170. Determination of the half life of thiocyanate in the plasma of Haemulon chrysargyreum (smallmouth grunt fish) exposed to potassium cyanide. **J. Brown**, H. Nolte, N.E. Breen, A. Rhyne

ANYL 171. Determination and speciation of arsenic in single rice grains using HG-AFS. **J. Sibbick**, C.L. Martin, J.F. Tyson

ANYL 172. Raman, TGA and DSC studies of non-ideal lipid mixtures. **N. Phambu**, B.M. Almarwani, A. Sunda-Meya

ANYL 173. Mechanisms of σ66RNAP: Scc4 mediated transcriptional regulation in *Chlamydia trachomatis*. **T. Ukwaththage**, L. Shen, M. Macnaughtan

ANYL 174. Sensor fusion for biological imaging. **J. Askim**, S. Semancik

ANYL 175. Electrochemical determination of surface area-to-volume ratio for metal nanoparticle size analysis. **J. Sharma**, D. Pattadar, B. Mainali, F.P. Zamborini

ANYL 176. Development of a paper analytical device for the detection of radon levels. **J. Zinna**, M. Lieberman

ANYL 177. Analyzing out-of-plane emission from gap mode SERS substrates. **A. Cutri**, P. Joshi, T.P. Anthony, A.J. Wilson, K.A. Willets

ANYL 178. Assessing legacy pollution by shell surface XRF analysis of sedentary shellfish. **S. Green**, S.K. O'Shea

ANYL 179. Antioxidant analysis of honey. **B. Esterlen**, **B.J. Bellott**

ANYL 180. Comparison of caffeine concentration in brewed teas. **Q. Kruel**, **B.J. Bellott**

ANYL 181. Functionalization of gold nanoparticles with aminooxy thiol ligands. **T.R. Sibakoti**, F.P. Zamborini, M.H. Nantz

ANYL 182. Application of BURBOP universal rotation pulses to ^{19}F 2D NMR experiments. **A.A. Marchione**, E. Diaz

ANYL 183. Electron transfer dissociation and collision-induced dissociation mass spectrometry of trivalent metal adducted oligosaccharides. **R. Duke**, C.J. Cassady

ANYL 184. Direct method for determining the concentrations of trace metals in aqueous samples using microwave plasma-atomic emission spectroscopy. **M.M. Gruber**, A.H. Coffman

ANYL 185. The rapid determination of controlled and non-controlled standards using direct analysis in real time (DART) coupled with the Thermo Q-Exactive. **M.a. Febo**

ANYL 186. An environment-sensitive fluorescent polyamino acid for fingerprint-based protein profiling. **S. Tomita**, S. Ishihara, R. Kurita

ANYL 187. Measuring levoglucosan in plasma using ICECLES method. **A. Kittelson**, J. Dzisam, B.A. Logue

ANYL 188. Isolation and identification of antimicrobial peptides from *Solanum lycopersicum*. **W. Evans**, T. Bartges, C.L. Kirkpatrick, L. Hicks

ANYL 189. Ligand controlled morphology evolution of gold nanostars. **J. Dyer**, X. Meng, C. Jiang

ANYL 190. Detection of adrafinil using electrochemical methods. **S.K. Conlin**, D.A. Fry

ANYL 191. Triggerable rapid contents release and fusion of redox sensitive quinone lipid-based liposomes. **H. Nguyen**, R.L. McCarley, J.E. Winter

ANYL 192. Reusable metal ion-imprinted polymer sponges for selective removal of heavy metals. **A.K. Seaux**, G. Canlas, R. Barbosa

ANYL 193. Incorporating green chemistry principles into analytical chemistry curriculum: Development of green HPLC methods for determination of renal function biomarkers in human fluids. **Y. Zuo**, S. Zhou, R. Zuo, X. Lu, Y. Deng

ANYL 194. A nanobionic light emitting plant. S. Kwak, J. Giraldo, M. Wong, **V. Koman**, T. Lew, R. Sinclair, W.A. Tisdale, M. Landry, M. Strano

ANYL 195. Ionic strength mediated phase transitions of adsorbed DNA on single-walled carbon nanotubes. D. Salem, X. Gong, A. Liu, **V. Koman**, J. Dong, M. Strano

ANYL 196. Determination of nicotine level in soil using HPLC/UV. **C. Dallimore**, **Y. Zhang**, **Q. Zhang**

ANYL 197. Single-molecule fluorescence competitive hybridization assay to detect unlabeled DNA at individual probe sites on surfaces. **W. Li**, E.M. Peterson, J.M. Harris

ANYL 198. Spectrophotometric determination of aluminum in human sweat using Alizarin Yellow R. **J. Walker**, K.T. Jackson

ANYL 199. Development of immunoassays for detecting oxyfluorfen residue in agricultural products. **E. Sheng**, **J. Hao**

ANYL 200. Evaluation of the effect of common cooking practices of rice on its metal content. **W.M. Alrawi**

ANYL 201. Purification of used vegetable oil using groundnut shell. **S.O. Ohenhenlen**, **A.A. Aliyu**, **O.O. Onawumi**

ANYL 202. Comparative studies of metal complexes of 5,10,15,20-tetrakis(2-(trifluoromethoxyphenyl)porphyrin and its isomers. **A. Adeyemo**

ANYL 203. Synthesis and characterization of new photosensitizers: Potential anti-HIV/cancer drugs. **A. Adeyemo**

ANYL 204. Confocal-Raman microscopy determination of temperature-dependent partitioning of PAHs in C_{18}-modified silica particles and interdigitated hybrid-bilayer particles. **X. Wen**, D. Bryce, J.P. Kitt, J.M. Harris

ANYL 205. Absorption of chromium via amino modified biochar. **K. Flores**, D. Gonzalez, J. Parsons

ANYL 206. Effects on alternating the concentration of the bases and temperature in Suzuki cross coupling reactions. **J.A. Perez**, D. Gonzalez, J. Parsons

ANYL 207. Fluoride removal with magnesium/aluminum modified biochar. **E.M. Powell**

ANYL 208. Characterization of the cigarette tar radical using ATR-IR and electrospray ionization mass spectrometry. A.R. Skochko, S. Russell, **K. Stone**

ANYL 209. Extraction of hydrophilic cosmetic components using hydrogels and surface enhanced Raman spectroscopy (SERS) detection. **R. Olson**, D. O'Donnell

ANYL 210. Sensitive chiral analysis of chiral isotopologues via microwave three-wave mixing. **L. Satterthwaite**, S. Eibenberger, C. Perez, R.L. Broadrup, D. Patterson

ANYL 211. Removal of chromium(III) and chromium(VI) from aqueous solution using $K_2Mn_4O_9$ under light conditions. **J. Valle**, J.M. Cantu, C. Valdes, D. Gonzalez, J. Parsons

ANYL 212. Determination of lead (Pb), barium (Ba), and antimony (Sb) in gunshot residue by thin film hydride generation microwave plasma atomic emission spectroscopy (MP-AES). **K. Lambert**, A.M. Scarton

ANYL 213. Comparative phytochemical analysis of *Citrullus ecirrhosus* and *Citrullus mucosospermus* using HPLC and LC-MS. **J. Swanier**, R.L. Jarret, J.T. Lyles, C.L. Quave

ANYL 214. Source attribution of dokha, a Middle Eastern tobacco product. **E. Hondrogiannis**, L. Frank, C. Wheeler, A. Belunis, R. Alibozek

ANYL 215. Toxic Moscow mules? Dangerous lipsticks? Analyzing the metal content in everyday items. **J.M. Wiester**

ANYL 216. Separation of biosimilars using a 2 µm silica based size exclusion chromatography column. **A. Chakrabarti**

ANYL 217. Correlating fatty acid composition of omega-3 fatty acids to antioxidant protection using a combination of gas chromatography-flame ionization detection and square wave voltammetry. **M.J. Fhaner**

ANYL 218. New approaches to 3D chemical mapping and electronic state analysis at low microns resolution. **W. Yun**, S. Lewis, B. Stripe, S. Seshadri, S. Lau

ANYL 219. Withdrawn

ANYL 220. Discrimination of carboxylate anions in neutral water using chemical fingerprinting methods. **Y. Xu**, M. Bonizzoni

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ANYL 221. Rapid detection of *Escherichia coli* by double cross-PRIMING amplification. X. Wang, S. Niu, C. Shi, **C. Ma**

ANYL 222. Rapid and efficient detection of mycoplasma pneumonia RNA by reverse-transcription loop-mediated isothermal amplification (RT-LAMP). **C. Ma**, C. Yan, C. Shi

ANYL 223. Applications of multidimensional time model for PDF applied to Brownian motion on fractals to solution of different questions of equilibrium, depolarization, filtering, memory friction, and different time scales and energy barriers in 1D Kramers' model for kinetics of chemical reactions and its 2D, 3D, and multi-D modifications and further application to surface acoustic wave pressure sensors. **M. Fundator**

ANYL 224. Investigation of the interactions between IRP and ferritin IRE. M. Miller, K. King, R. Clark, M. Kimble, E. Mendenhall, **B. Wang**

ANYL 225. A potentiometric solid contact micro-sensor to monitor intake of zinc ions in plants. **K.Y. Chumbimuni Torres**, S.M. Armas

ANYL 226. Electrochemical studies of Si(111) surfaces functionalized with hybrid nanomaterials. **F. Konopka**, M.J. Rose

ANYL 227. Open characterization of e-cigarette refill fluids and quantitative determination of selected analytes of concern. **N. Mladjenovic**

ANYL 228. Selective and sensitive detection of pathogens with pathogen-imprinted polymers. **M. Dulay**

ANYL 229. Polymer-spray mass spectrometry for rapid analysis of drugs in biofluids. **M. Dulay**

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 228

Biomolecular, Molecular & Elemental Spectrometry with Plasma Sources

Financially supported by Meinhard; Thermo Fisher Scientific
J.T. Shelley, *Organizer*
G.M. Hieftje, *Organizer, Presiding*
J. Shelley, *Presiding*

8:30 ANYL 230. Novel plasma-based tools for real-time mass-spectral analysis of atomic, molecular, and polymeric species. **J.T. Shelley**, A.J. Schwartz, C.L. Walton, S.P. Badal, G.M. MacLean, M.J. Burnley, J. Wu, J.R. Hellinger, G.M. Hieftje

9:00 ANYL 231. Elemental and molecular mass spectrometry development for biological and environmental science. **D.W. Koppenaal**, R.M. Boiteau, L. Pasa-Tolic, E. Hoegg, R.K. Marcus

9:30 ANYL 232. Method development for metal detection at cellular levels by ICP-MS. **N. Jakuboski**

10:00 ANYL 233. Optical isotopic analysis with laser-induced plasma. **G. Chan**, X. Mao, V. Zorba, R. Russo

10:30 Intermission.

11:00 ANYL 234. Liquid sampling-atmospheric pressure glow discharge (LS-APGD) microplasma: A combined atomic and molecular (CAM) ionization source. **R.K. Marcus**, D.W. Koppenaal, E. Hoegg, T. Williams

11:30 ANYL 235. Perspectives for analytical chemistry: From single nanoparticle detection with ICP-MS to nanotoxicology studies in aquatic ecosystems. **C. Engelhard**, D. Mozhayeva, I. Strenge, B. Spelz, H. Schonherr, B. Steinhoff, K. Witte, S. Hartmann, K. Kuhnert, J. Kunze, C. Schlechtriem, R. Zeumer, J. Wanzenböck, D. Lamatsch, R. Vogt, S. Loureiro, V. Galhano, M. Monteiro, I. Lopes

12:00 ANYL 236. Is there no better analytical plasma source than the ICP? **G.M. Hieftje**

Section B
Ernest N. Morial Convention Center
Room 230

Analytical Chemistry in the Developing World

Environmental Applications

Cosponsored by MPPG‡
C.J. Brady, T. Cleary, M. Lieberman, *Organizers*
A. Cooper, *Organizer, Presiding*
M. Dowd, *Presiding*

8:30 Introductory Remarks.

8:35 ANYL 237. Learning from water catastrophes of the world. **S. Ahuja**

9:05 ANYL 238. Portable low-cost instrumentation for metallic colloid scattering chemical sensors of water contaminants. G. Vasquez, Y. Hernandez, **Y. Coello**

9:25 ANYL 239. Electrochemical detection of *E. coli* enzyme activity for improved point-of-use bacterial water testing in resource-limited environments. **M.S. Bono**, E. Hanhauser, S. Beasley, C. Vaishnav, A. Hart, R. Karnik

9:45 ANYL 240. Detoxification of waste water of Pb^{2+} and Cd^{2+} using agricultural waste of boiled groundnut(*arachis hypogaea*) shells. **T.A. Abii**

10:05 Intermission.

10:10 ANYL 241. Analytical chemistry in developing urban environments: Lessons from New Orleans. **H.W. Mielke**

10:40 ANYL 242. Long-range physical transport and in-situ chemical transformation of atmospheric aerosols: Case studies in western Africa, the Caribbean and eastern Asia. **S. Gao**

11:10 Panel Discussion.

Section C
Ernest N. Morial Convention Center
Room 229

Ultrafast Spectroscopy Meets Chemistry, Materials & Biology

Multidimensional Spectroscopy

K.W. Huang, I.V. Rubtsov, J. Zheng, *Organizers, Presiding*

8:30 ANYL 243. Triplet dynamics during singlet fission in functionalized pentacenes examined with ultrafast vibrational spectroscopy. **J.B. Asbury**

9:05 ANYL 244. Ultrafast 2D IR spectroscopy of lipid membranes: Experiments and simulations. M. Valentine, **C.R. Baiz**

9:40 ANYL 245. Investigating 2D materials and van der Waals heterostructures with ultrafast infrared microspectroscopy. **H. Chen**, X. Wen, W. Zhuang, G. Zhang, J. Zheng

10:15 Discussion.
10:25 Intermission.

10:40 ANYL 246. Ultrafast dynamics of photosynthetic energy transfer regulated by intrinsic redox reactivity of amino acid side chains in binding pocket. M.A. Allodi, J.P. Otto, S.H. Sohail, R. Saer, R.E. Wood, B.S. Rolczynski, S.C. Massey, P. Ting, R.E. Blankenship, **G.S. Engel**

11:15 ANYL 247. Mechanism of action of biological cosolvents revealed by ultrafast vibrational dynamics. **F. Gai**

11:50 ANYL 248. 2D IR spectroscopic studies of 5-cyano-tryptophan. **F. Chalyavi**, P.H. Gilmartin, M.W. Fennie, M.J. Tucker

Section D
Ernest N. Morial Convention Center
Room 227

Wearable & Implantable Sensors
Cosponsored by MPPG‡
M.A. Daniele, L. Deravi, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ANYL 249. Flexible multi-analysis electronics: Perception of human self. **F. Li**

8:55 ANYL 250. Studies toward developing a wearable breath sensor for detecting hypoglycemia using VOCs. **M. Agarwal**, A. Daneshkhah, A. Siegel, S. Vij, I. Momoh

9:15 ANYL 251. Harnessing the biochemical energy of glucose. **G. Slaughter**

9:35 ANYL 252. Ultrathin, flexible, and injectable biosensors. **A. Koh**

9:55 ANYL 253. Electrochemical, aptamer-based sensing enables closed-loop control of plasma drug levels directly in live animals. **N. Arroyo**

10:15 Intermission.

10:30 ANYL 254. Going where few wearables dare to go: Injectable, tissue-integrating biosensors for long-term, continuous monitoring of body chemistries. **N.A. Wisniewski**

11:00 ANYL 255. Polymer code for strategic design of tissue-like materials. **S. Sheiko**

11:30 ANYL 256. Polymeric peptide pigments with sequence-encoded properties. **A. Lampel**, S. McPhee, H. Park, G. Scott, S. Humagain, D. Hekstra, B. Yoo, P. Frederix, T. Li, R. Abzalimov, S. Greenbaum, T. Tuttle, T. Hu, C. Bettinger, R. Ulijn

Section E
Ernest N. Morial Convention Center
Room 226

Ionic Liquids: Recent Trends & Applications

W.L. Hinze, C.D. Tran, I.M. Warner, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 ANYL 257. Ionic liquids in separations and mass spectrometry. **D.W. Armstrong**

9:10 ANYL 258. Ionic liquids and bio resources: Several opportunities are still possible. **C. Chiappe**, L. Guazzelli, C.S. Pomelli

9:40 ANYL 259. Ionic liquids for controlled synthesis of functional materials for applications in analytical chemistry. **S. Dai**

10:10 Intermission.

10:25 ANYL 260. Ionic liquids and GUMBOS: Tunable materials for biomedical applications. **I.M. Warner**

10:55 ANYL 261. Advanced biodegradable/biorenewable sorbents for uranium extraction from seawater. **R.D. Rogers**, G. Gurau

11:25 ANYL 262. Total green synthesis of silver nanoparticle composites. **C.D. Tran**

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 228

Analytical Chemistry of Biofuels
Cosponsored by MPPG‡
Financially supported by Falcon Analytical; Infometrix Inc; The College of the Holy Cross
A.M. Hupp, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ANYL 263. Elucidating structural characteristics of renewable products from a two-step ex situ hydropyrolysis vapor upgrading process by one- and two-dimensional NMR spectroscopy. **J. Lai**, L. Zhang, K. Gong

2:05 ANYL 264. HPAE-PAD method for determination of sugars in algal biomass. **S. Patil**, M. Tran-Gyamfi, R.W. Davis, J. Rohrer

2:35 ANYL 265. Triacylglycerol-based fuels: An evaluation. **G. Knothe**

3:05 Intermission.

3:20 ANYL 266. Mobile compact ^{1}H NMR spectroscopy for on-line monitoring of the biodiesel production reaction. D. Galvan, L. Magalhães de Aguiar, D. Borsato, J.J. Rohwedder, **M.H. Killner**

3:50 ANYL 267. Chromatography and chemometric analysis of biodiesel fuel blends. **K.M. Pierce**

4:20 ANYL 268. Determination of biodiesel concentration and feedstock using ultrafast GC, PCA, and PLS. **A.M. Hupp**, J. Perron, N. Roques, J. Crandall, S. Ramos, B. Rohrback

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4:50 ANYL 269. Fatty acid profile of alternative feedstocks for biodiesel production and implications for fuel properties. **B.R. Moser**

Section B
Ernest N. Morial Convention Center
Room 230

Analytical Chemistry in the Developing World

Food & Nutrition

Cosponsored by MPPG‡
C.J. Brady, T. Cleary, A. Cooper, M. Lieberman, *Organizers*
V. Henry deFrahan, *Presiding*

1:30 Introductory Remarks.

1:35 ANYL 270. Combating food fraud in the developing world with analytical chemistry. **J. Almirall**

2:05 ANYL 271. Development of a test-kit method for the determination of arsenic in rice in Bangladesh. **J.F. Tyson**, N. Fragola, I. Rafiyu

2:35 ANYL 272. Colorimetric sensor arrays for biomedical applications. **K.S. Suslick**, Z. Li

3:05 Intermission.

3:10 ANYL 273. Deciphering signaling pathways controlling metabolism in *Chlamydomonas reinhardtii*. **L.M. Hicks**

3:40 ANYL 274. Progress in the monitoring of chemical residues in food. **S.J. Lehotay**

4:10 Panel Discussion.

Section C
Ernest N. Morial Convention Center
Room 229

Ultrafast Spectroscopy Meets Chemistry, Materials & Biology

Imaging

K.W. Huang, I.V. Rubtsov, J. Zheng, *Organizers, Presiding*

1:30 ANYL 275. Quantitative ultrafast imaging from quantum dots to tissues. **M. Gruebele**

2:05 ANYL 276. Real-time 3D single-particle tracking spectroscopy: Development and applications. **H. Yang**

2:40 ANYL 277. Novel ultrafast laser ablation sampling technologies in optical emission elemental and isotopic imaging. **V. Zorba**

3:15 Intermission.

3:30 ANYL 278. Second-order spectral lineshapes from charged interfaces. **F. Geiger**

4:05 ANYL 279. Understanding the origins of ultralong radiative states in metal halide perovskite crystals. E. Alarousu, A. El-Zohry, K. Lee, B. Turedi, I. Dursun, J. Yin, A. Zhumekenov, S. Mitra, I.S. Roqan, C. Yang, A. Malko, O. Mohammed, **O.M. Bakr**

4:40 ANYL 280. Interaction of spin and orbital angular momentum of light with bulk GaAs. **P. Navotnaya**, B. Rolczynski, G.S. Engel

Section D
Ernest N. Morial Convention Center
Room 227

Wearable & Implantable Sensors
Cosponsored by MPPG‡
L. Deravi, *Organizer*
M.A. Daniele, *Organizer, Presiding*
M. Yokus, *Presiding*

1:30 ANYL 281. Microfabrication of epidermal multiplexed sensors for glucose, lactate and pH. **M. Yokus**, V. Pozdin, M. Wilkins, M.A. Daniele

1:45 ANYL 282. Implantable hydraulic sensor to monitor tibial plate bending in fracture healing process with standard radiography. **A. Rajamanthrilage**, H. Pelham, P.W. Millhouse, M. Arifuzzaman, N. Carrington, C. Behrend, J.D. DesJardins, J.N. Anker

2:00 ANYL 283. Ultra-sensitive, highly-selective, real-time chemical sensors based on hydrogel interferometer. **M. Sun**, X. Yang, J. Song, X. He

2:15 ANYL 284. Phthalocyanine GUMBOS for discrimination of VOCs using a quartz crystal microbalance based multisensor array. **S. Vaughan**, N. Speller, P. Chhotaray, N. Siraj, K.S. McCarter, R.L. Perez, I.M. Warner

2:30 Intermission.

2:45 ANYL 285. Using dye-doped polymer and phosphor based coatings to image surface specific changes in pH on implanted medical devices through tissue. **U. Uzair**, J.N. Anker

3:00 ANYL 286. Wearable potentiometric sensors for heavy metals detection. **M. Rostampour Kakroudi**, S.M. Armas, K.Y. Chumbimuni Torres

3:30 ANYL 287. ZnO nanostructure-based linker-free biosensors for alcohol and lactate sensing in sweat. **F. Alam**, A.H. Jalal, Y. Umasankar, N. Pala

3:45 ANYL 288. Multivariate analysis method for precise measurement of volatile compounds by wearable sensors. **A.H. Jalal**, Y. Umasankar, S. Kedia, R. Matos, S. Bhansali

4:00 ANYL 289. Purine precursor detection for pre-symptomatic diagnosis of wounds. **S. RoyChoudhury**, **Y. Umasankar**, S. Bhansali

4:15 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 226

Ionic Liquids: Recent Trends & Applications

W.L. Hinze, C.D. Tran, I.M. Warner, *Organizers, Presiding*

1:30 ANYL 290. Fabrication of renewable biocomposite materials using Ionic liquid based methods. **P.C. Trulove**, D.P. Durkin, A. Burn, P. Fahey, S. Park, R. Chung, L. Haverhals, H. De Long

2:00 ANYL 291. Advances in the synthesis of high-performance fuel cell membranes using innovative radiation grafting techniques on fluorinated hydrocarbon polymeric substrates: from styrene to ionic liquids. **D. Poster**, K. Mecadon, Z. Tsinas, J. Robertson, M. Postek, M. Al-Sheikhly

2:30 ANYL 292. Beyond petroleum-based plastics: Characterizations of functional fiber welded biocomposite materials. **L.M. Haverhals**, D.P. Durkin, H. Mitiku, J. Choi, X. Tang, A. Amstutz, H.C. De Long, P.C. Trulove

3:00 Intermission.

3:15 ANYL 293. Potential impact of ionic liquids in the field of additive manufacturing. **W.M. Reichert**, G.M. Poole, T.R. Ellett

3:45 ANYL 294. Chiral ionic liquids derived from *L*- valine as chiral solvents and selectors for enantiomeric recognition. **D. Bwambok**

4:05 ANYL 295. Enhancing photo-physical properties of propidium iodide by substitution of organic anions. **T.P. De Silva**, B. Yang, I.M. Warner

4:25 ANYL 296. Specific conductivity and viscosity of imidazolium-based ionic liquid: Effect of co-solvents. **M. Thakurathi**, V. Thalangamaarachchige, E.L. Quitevis

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern
Sponsored by ENVR, Cosponsored by ANYL and CEI

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

Undergraduate Research Posters

Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix

L.A. Baker, *Organizer*

8:00–10:00

64, 66-67, 69, 71-73, 77, 80-81, 83, 85, 92, 106, 108, 116, 119, 123, 126, 129, 130, 132, 134, 143, 148-149, 150, 157, 159, 162, 166, 169, 171, 175-176, 178, 183-185, 191, 193, 197, 210, 215-216, 227, 229. See previous listings.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 228

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Jani C. Ingram
Cosponsored by PROF and WCC
R.D. Foust, *Organizer, Presiding*

8:30 Introductory Remarks.
8:40 ANYL 297. Award Address
(ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences Sponsored by The Camille and Henry Dreyfus Foundation, Inc.). Engaging Native American students in environmental health studies on contaminated lands. **J.C. Ingram**

9:20 ANYL 298. Native environmental health research (NEHR) network: Developing collaborative service-oriented analytical research for Native American students. **D. Stevens**

9:50 Intermission.

10:05 ANYL 299. Professor Jani Ingraam at the Northern Arizona University Chemistry Department has been focused on substanially increasing the representation of Native American students in science research through current issues of uranium contamination on the Navajo Reservation. **L. Edgewater**

10:35 ANYL 300. Creating opportunities for disadvantaged undergraduate students in nuclear chemistry: Forensic studies of uranium sources in the environment. **M.E. Ketterer**

11:05 ANYL 301. Environmental arsenic studies as a way to introduce undergraduates to research. **R.D. Foust**

Section B
Ernest N. Morial Convention Center
Room 230

Analytical Chemistry in the Developing World

Applications in Medicine

Cosponsored by MPPG‡
T. Cleary, M. Lieberman, *Organizers*
C.J. Brady, A. Cooper, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ANYL 302. Addressing the 3A's (availability, accountability, adherence) of supply chain systems in western Kenya. **M. Maina**, R. Karwa, D.N. Tran, B. Njuguna, I. Manji, P. Wasike, E. Tonui, G. Kigen, M. Lieberman, S. Pastakia

9:05 ANYL 303. Development of a paper analytical device to access quality of chemotherapy drugs. **M.D. Smith**

9:25 ANYL 304. Paper-based microfluidics for emerging disease detection. **C. Henry**, B. Geiss, K. Boehle, R.B. Channon, C. Carrell

9:55 Intermission.

10:00 ANYL 305. Antibiotic resistance gene detection through sequence-specific extraction using DNA-modified porous polymer monoliths. **A. Woolley**, R.L. Hanson, B.R. Peine, R. Knob

10:30 ANYL 306. Withdrawn

10:50 Panel Discussion.

Section C
Ernest N. Morial Convention Center
Room 229

Ultrafast Spectroscopy Meets Chemistry, Materials & Biology

Interfaces

‡*Cooperative Cosponsorship*

K.W. Huang, I.V. Rubtsov, J. Zheng, *Organizers, Presiding*

8:30 ANYL 307. Ultrafast processes in nano, molecular, & hybrid semiconductors. **X. Zhu**

9:05 ANYL 308. Probing vibrational-electronic coupling at interfaces via doubly-resonant sum frequency spectroscopy. S. Sengupta, D.W. Elsenbeck, M. Raab, **L.A. Velarde**

9:40 ANYL 309. Tracking ultrafast charge carrier dynamics at the interface of perovskite nanocrystals using time-resolved laser spectroscopy. **O. Mohammed**

10:15 Discussion.
10:20 Intermission.

10:35 ANYL 310. Monolayer dynamics at the air/water interface: From ultrafast to ultraslow dynamics. **M.D. Fayer**

11:10 ANYL 311. In situ vibration sum frequency generation spectroscopic probe of molecular structures and dynamics at electrochemical interfaces. **T. Lian**

11:45 ANYL 312. Probing the mechanism of charge transfer in organic crystals using femtosecond stimulated Raman spectroscopy. **A.A. Cassabaum**, W. Silva, R.R. Frontiera

Section D
Ernest N. Morial Convention Center
Room 227

Advances in Blood-Based Diagnostics

R.A. Dluhy, M.D. Porter, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ANYL 313. Zwitterion-functionalized PEI/PVA nanofibers embedded in a microfluidic chip for efficient capture and intact release of circulating tumor cells. **Y. Xiao**, M. Wang, L. Lin, L. Du, M. Shen, X. Shi

9:10 ANYL 314. Raman hyperspectroscopy for disease diagnostics and forensic phenotype profiling. **I.K. Lednev**

9:45 ANYL 315. SERS detection of cancer biomarkers. J. Li, H. Cheng, **C. Zhong**

10:20 Intermission.

10:40 ANYL 316. Extracellular vesicles (EVs) as blood-based markers: Microfluidics for their enrichment and analysis. **S.A. Soper**

11:15 ANYL 317. Nanoscale infrared spectroscopy and imaging of aging red blood cells. **C.A. Marcott**, S. Ruggeri

11:50 ANYL 318. Detection of the tuberculosis antigenic marker lipoarabinomannan in infected patient sera by gold nanoparticle labeling and surface-enhanced Raman scattering. **M.D. Porter**

Section E
Ernest N. Morial Convention Center
Room 226

Advancements in Bio-Recognition Element Discovery & Development & Its Translation into Innovative Biosensor Technologies

S. Kim, B. Lee, T. Ulep, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ANYL 319. Development of phage-based nanobots for the recognition, separation, and detection of bacterial pathogens. T. Hinkley, E.M. Pulkkinen, E. Farquharson, M.M. Duong, J. Talbert, **S.R. Nugen**

9:00 ANYL 320. Biosensing applications incorporating synthetic DNA molecules with catalytic and binding properties. **Y. Li**

9:25 ANYL 321. Screening of pairs of aptamers to nanobiosensors and lateral flow assays. **M. Gu**

9:50 ANYL 322. Identification of biorecognition elements specific to biomarkers through a combination modeling, *in vitro* and, high throughput microarray methods. **R. Krabacher**, Y. Chushak, P. Mirau, S. Larson, J.L. Chavez, N. Kelley-Loughnane

10:05 Intermission.

10:15 ANYL 323. Real-time Biosensors for continuous measurements of specific biomolecules in live animals. **H.T. Soh**

10:40 ANYL 324. BioDot, Inc. provides non-contact low volume dispensing solutions valuable in the biosensor industry. **C. Fronczek**

11:05 ANYL 325. Plasmonic "Ojogel" kit for detecting corneal integrity post glaucoma surgery. **S.K. Misra**, K. Dighe, Z. Shang, L. Labriola, D. Pan

11:20 ANYL 326. Early diagnosis of periodontal diseases using an aptamer-based biosensor with enhanced sensitivity. **B. Lee**, Y. Ko, J. Park, S. Ji, M. Gu

11:35 ANYL 327. Defect engineered TiO_2 nanotube photonic crystals for fabrication of near-infrared photoelectrochemical sensor. **W. Wu**

11:50 Concluding Remarks.

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, ENVR‡, INOR, PMSE‡ and PRES‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 228

ACS Award in Chromatography: Symposium in honor of Janusz Pawliszyn

P. Ross, *Organizer, Presiding*
1:30 Introductory Remarks.

1:35 ANYL 328. Biocompatible solid phase micro extraction, shaping the future for biological sampling isolation. **C. Aurand**, E. Barrey, D.S. Bell

2:15 ANYL 329. How can SPME help in decision making process in clinical practice? **B.G. Bojko**

2:55 ANYL 330. Know the true efficiency of your HPLC column despite the detector ruining it. **P.K. Dasgupta**

3:35 Intermission.

3:50 ANYL 331. Magnetic ionic liquids as extraction and preservation solvents for nucleic acid sample preparation. **J.L. Anderson**, K.D. Clark, O. Nacham, M. Varona

4:30 ANYL 332. Award Address (ACS Award in Chromatography Sponsored by MilliporeSigma). Think big but design small: A path for green analytical chemistry for next generations. **J.B. Pawliszyn**

Section B
Ernest N. Morial Convention Center
Room 230

Analytical Chemistry in the Developing World

Technology Development

Cosponsored by MPPG‡
C.J. Brady, T. Cleary, A. Cooper, M. Lieberman, *Organizers*
C. Stanton, M. Tetrick, *Presiding*

1:30 Introductory Remarks.

1:35 ANYL 333. Out of the lab and into the world. **M. Lieberman**

2:05 ANYL 334. Excel and high performance electronics: A powerful alternative to commercial instrumentation. **S. Abbott**

2:25 ANYL 335. Building a compact and simple surface-enhanced Raman spectroscopy platform that enables rapid on-site detection of coffee metabolites beyond nanomole level. **B.C. Galarreta**, A. Saldaña Ramos, Y. Hernández García, L. Ayala Correa, L. Lagos

2:45 ANYL 336. A portable and reusable colorimetric sensor for carcinogenic aromaic amines *via* interface regulation of graphene-enzyme hybrids. **Z. Qu**, M. Zhang, G. Shi

3:05 Intermission.

3:10 ANYL 337. Withdrawn

3:35 ANYL 338. Improving electrophoretic separations using A parafilm-paper-based analytical platform. **J. Mettakoonpitak**, C. Henry

3:55 ANYL 339. Organic solar power integrated greenhouses: Challenges and opportunities. **B. O'Connor**, H.W. Ade, W. You

4:25 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 229

Ultrafast Spectroscopy Meets Chemistry, Materials & Biology

Plasmonics: Materials, including 2D materials

K.W. Huang, I.V. Rubtsov, J. Zheng, *Organizers, Presiding*

1:30 ANYL 340. Plasmonic enhancement of selective virus inactivation through femtosecond laser irradiation. M. Nazari, S. Erramilli, **B.M. Reinhard**

2:05 ANYL 341. 2DIR spectroscopy of molecules under plasmonic fields: Towards understanding the 2D Fano line shapes and signal enhancement mechanisms. **L. Chuntonov**

2:40 ANYL 342. 2D IR vibrational energy transfer between azido- and cyano- reporters in different molecular scaffolds. **M.J. Tucker**

3:15 Intermission.

3:25 ANYL 343. Ultrafast tabletop XUV absorption spectroscopy of transition metal complexes and organohalide perovskites. **J. Vura-Weis**

4:00 ANYL 344. Probing photoexcited charge dynamics of single oxygen vacancies on TiO_2(110) at atomic scale. **Y. Jiang**

4:35 ANYL 345. Engineering of the surface and interface of monolayer MoS_2. **G. Zhang**

5:10 ANYL 346. Dual-frequency surface-enhanced two-dimensional vibrational spectroscopy of thin layers at an interface. **R.T. Mackin**, B. Cohn, L. Chuntonov, I.V. Rubtsov

Section D
Ernest N. Morial Convention Center
Room 227

Advances in Blood-Based Diagnostics

R.A. Dluhy, M.D. Porter, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ANYL 347. Withdrawn

2:10 ANYL 348. Online SERS characterization of serum. E. Peters, C. Wang, J. Li, **Z.D. Schultz**

2:45 ANYL 349. SERS based predictive assay for the treatment of prostate cancer. **M.T. McDermott**, S. Rajput

3:20 Intermission.

3:40 ANYL 350. Investigating antibody adsorption dynamics onto gold nanoparticles to form stable conjugates for analysis of biological fluids. **J.D. Driskell**, G. Ruiz, K. Tripathi

4:15 ANYL 351. Direct biochemical characterization of stored red blood cells using Raman spectroscopy. R. Gautham, J. Oh, R. Patel, **R.A. Dluhy**

Section E
Ernest N. Morial Convention Center
Room 226

Advancements in Bio-Recognition Element Discovery & Development & Its Translation into Innovative Biosensor Technologies

S. Kim, B. Lee, T. Ulep, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ANYL 352. Quantum plasmonics and its applications in life sciences and medicine. **L. Lee**

2:00 ANYL 353. Wearable biosensors for human performance monitoring: Challenges and considerations for device development. **A. Nicolini**

‡*Cooperative Cosponsorship*

2:25 ANYL 354. Biomolecular engineering of redox enzymes: Alteration of the electron acceptor preference; from oxygen to direct electron transfer. **K. Sode**

2:50 ANYL 355. Ratiometric fluorescence nanoprobe for hydroxyl radical detection. **M. Cong**, N. Siraj, N. Bhattarai, P.E. Kolic, K.S. McCarter, P. Chhotaray, I.M. Warner

3:05 ANYL 356. Enhancing the sensitivity using a nanostructured surface of the electrode functionalized with nature-derived material and aptamer pair. **S. Kim**, M. Gu

3:20 ANYL 357. GelRed/$[G_3T]_5$/Tb^{3+} hybrid: A novel label-free ratiometric fluorescent probe for H_2O_2 and oxidase-based visual biosensing. **J. Chen**

3:35 Intermission.

3:45 ANYL 358. A semi-synthetic organism that stores and retrieves increased genetic information. **F.E. Romesberg**

4:10 ANYL 359. Amplification-free detection of nucleic acids and proteins by electrokinetic concentrator. **W. Ouyang**, J. Han

4:25 ANYL 360. Peptide-mediated nanopore detection of uranyl ions in aqueous media: Environmental application. **G. M Roozbahani**, X. Guan, X. Chen, Y. Zhang

4:40 ANYL 361. Real-time quantification of droplet isothermal nucleic acid amplification through measurements of interfacial effects. **T. Ulep**, A. Day, J. Yoon

4:55 ANYL 362. Nanopore based DNA mismatch detection by single-strand-specific nuclease. **X. Chen**, G. M Roozbahani, Y. Zhang, X. Guan

5:10 ANYL 363. One-step assay for detection of HIV virus with sample-in-answer-out capability. S. Liu, S. Kuang, C. Shi, **C. Ma**

5:25 Concluding Remarks.

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, INOR, PHYS‡, PMSE‡ and PRES‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY EVENING

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COMP and PMSE

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 228

ACS Award in Analytical Chemistry: Symposium in honor of Michael L. Gross

L. Jones, *Organizer, Presiding*

8:30 ANYL 364. Targeted quantitative proteomic approaches for interrogating the human kinome. **Y. Wang**

9:10 ANYL 365. Native-ESI and ion mobility-mass spectrometry: Expanding MS-based structural biology through understanding of chemical fundamentals. **D.H. Russell**

9:50 ANYL 366. Extension of hydroxyl radical-based footprinting coupled with mass spectrometry for in cell and *in vivo* protein analysis. **L. Jones**

10:30 ANYL 367. Mass spectrometric studies on photosynthetic pigment-protein complexes. **R.E. Blankenship**

11:10 ANYL 368. Award Address (ACS Award in Analytical Chemistry Sponsored by the Battelle Memorial Institute). Mass spectrometry-based structural proteomics solves problems in biochemistry and bio-therapeutics. **M.L. Gross**

Section B
Ernest N. Morial Convention Center
Room 230

Biomedical Advances in Cancer Detection & Treatment Using Advanced Analytical Techniques

C. Burton, Y. Ma, *Organizers*
C. Burton, *Presiding*

8:30 Introductory Remarks.

8:35 ANYL 369. Assessing volatile organic compound biomarkers of prostate cancer found in urine headspace by gas chromatography/mass spectrometry. **M. Agarwal**, A. Siegel, A. Daneshkhah

8:55 ANYL 370. GC-MS analysis of volatile organic compounds in urine of mice with breast cancer, with treated breast cancer, and without breast cancer. **S. Naumann**, S. Liu, M. Teli, A. Siegel, H. Yokota, M. Agarwal

9:15 ANYL 371. Withdrawn

9:35 ANYL 372. Noninvasive characterization of epithelial cancers using a composite panel of urinary pteridines and modified nucleosides. **C. Burton**

9:55 Intermission.

10:10 ANYL 373. Manipulation of functional parameters of plasmon-based sensor for effective microRNA assay in patient plasma. **T. Habarakada Liyanage**, R. Sardar, H.z. Kaimakliotis

10:30 ANYL 374. Novel mitochondria-targeted fluorescent probes (MitoProbes) for detection of mitochondrial reactive oxygen species (mtROS) generation. **S. Hou**

10:50 ANYL 375. Selective chemotherapeutic applications of rhodamine-based NanoGUMBOS. **N. Bhattarai**, I.M. Warner, M. Chen

11:10 ANYL 376. Design of novel heptamethine dye-based NanoGUMBOS as potential cancer therapeutics. **M. Chen**, N. Bhattarai, M. Cong, R.L. Perez, I.M. Warner

11:30 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 229

Novel Approaches to Mass Spectrometry Imaging

K.K. Murray, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ANYL 377. Robotic surface analysis mass spectrometry (RoSA-MS) of three-dimensional objects. **F.M. Fernandez**, A. Li, M. Paine, S. Zambrzycki, R. Bennett, M. Bouza

9:00 ANYL 378. Combining the single-probe mass spectrometry imaging with advanced data analysis. X. Tian, G. Zhang, Y. Shao, **Z. Yang**

9:25 ANYL 379. Laserspray ionization mass spectrometry: Fundamentals, instrumentation, and imaging applications. **S. Trimpin**

9:50 ANYL 380. Chemical imaging mass spectrometry: A universal, quantitative, rapid tool for discovery of biomarkers, IED classification and brain mapping. **R.J. Levis**

10:15 Intermission.

10:35 ANYL 381. Metal-assisted LDI for high resolution imaging MS of neutral lipids from thin tissue sections. **P. Chaurand**

11:00 ANYL 382. Laser Microdissection directly coupled with mass spectrometry for chemical imaging and spatially resolved qualitative and quantitative analysis. **G.J. Van Berkel**, J.F. Cahill, V. Kertesz

11:25 ANYL 383. MALDI MSI directed-infrared laser microsampling for tissue proteomics. K. Wang, **F. Donnarumma**, C. Szot, M.E. Pettit, T. Solouki, K.K. Murray

Section D
Ernest N. Morial Convention Center
Room 227

Comprehensive Chemical Characterization of Hydraulic Fracturing Shales, Wastes & Recycled Waste Products
Cosponsored by MPPG‡
J. Kucklick, *Organizer*
S. Christopher, *Organizer, Presiding*
D. Mueller, *Presiding*

8:30 Introductory Remarks.

8:35 ANYL 384. Continuing research to identify and address environmental and human health risks associated with the alternative management of oil and gas wastewater. **C. Danforth**, D. Mueller, N. Saunders

9:05 ANYL 385. Toxicity identification evaluation of produced waters of different production ages. **B.W. Brooks**, G. Saari, K. Kroll, N.D. Denslow

9:35 ANYL 386. Forward osmosis as an effective treatment technology for high salinity produced water from unconventional oil and gas development. **T. Liden**, D.D. Carlton, Y. Ide, T. Otoyo, N. Kubota, K. Schug

10:05 ANYL 387. Accessing information for chemicals in hydraulic fracturing fluids using the US EPA CompTox Chemistry Dashboard. **A.J. Williams**, A. McEachran, J. Sobus, C. Grulke, A. Richard

10:35 Intermission.

10:50 ANYL 388. Non-target mass spectrometry profiling of organic compounds in hydraulic fracturing flowback water. **C. Sun**, Y. Zhang, J.W. Martin, D. Alessi

11:20 ANYL 389. Discovery of proprietary amino ethoxylates in hydraulic fracturing wastewater using LC/Q-TOF/MS with solid phase extraction. **K. Sitterley**, K. Linden, I. Ferrer, E.M. Thurman

11:50 ANYL 390. Development and chemical characterization of a hydraulic fracturing wastewater reference material. **S. Christopher**, D. Bearden, C. Davis, K. Huncik

12:20 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 226

Advances in Separations

K. Phinney, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ANYL 391. Quantitative measurement of furfural, 5-hydroxymethylfurfural, N-methyl-2-pyrrolidone, benzene, and hydrogen cyanide metabolites in urine using UPLC-MS/MS. **D. Bhandari**, D. McCarthy, C. Movassaghi, V. De Jesús, B. Blount

9:00 ANYL 392. Laser ablation sampling of formalin fixed paraffin embedded tissue. K. Wang, **F. Donnarumma**, C. Szot, M.E. Pettit, T. Solouki, K.K. Murray

9:25 ANYL 393. Withdrawn

9:50 Intermission.

10:10 ANYL 394. Improvements to a UPLC-MS/MS method for simultaneous determination and quantification of 28 urinary biomarkers of volatile organic compound exposure. **C. Movassaghi**, D. Bhandari, D. McCarthy, D. Milan, V. De Jesús, B. Blount

10:35 ANYL 395. Nanofluidic interfaces for time resolved imaging of cellular metabolites. **D. Ediriweera**, L.J. Millet, P. Shankles, S. Retterer, M.J. Doktycz

11:00 ANYL 396. Nanofluidic system for desalination and solvent removal from water sources. **K. Rangharajan**, P. Mohanasundaram, A. Conlisk, S. Prakash

Inaugural Joint Symposium of the Separation Science Subdivisions
Sponsored by I&EC, Cosponsored by ANYL

Inaugural Joint Symposium of the Separation Science Subdivisions
Sponsored by I&EC, Cosponsored by ANYL

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 228

ACS Award for Research at an Undergraduate Institution: Symposium in honor of Joseph J. Pesek

‡*Cooperative Cosponsorship*

T.J. Wenzel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 ANYL 397. Beyond traditional liquid chromatography – mass spectrometry: Using the tools we now have and should use. **K. Schug**

2:20 ANYL 398. Polymer brushes as bonded phases for LCMS of protein drugs. **M.J. Wirth**, T. Chen, R. Jacobson

3:00 Intermission.

3:15 ANYL 399. Capillary electrophoresis as a tool for bottom-up proteomics. Z. Zhang, L. Sun, O. Krokhin, **N.J. Dovichi**

3:55 ANYL 400. Award Address (ACS Award for Research at an Undergraduate Institution Sponsored by the Research Corporation for Science Advancement). The history of silica hydride stationary phases for high performance liquid chromatography from conception to commercialization. **J.J. Pesek**

Section B
Ernest N. Morial Convention Center Room 230

Advances in Spectroscopy

J.M. Harris, *Organizer*
S.R. Emory, *Presiding*

1:30 ANYL 401. "Scattered" thoughts on understanding the interfaces of nanoparticle dispersions. **A. Carpenter**, G.L. Richmond

1:55 ANYL 402. Second harmonic and sum frequency generation from aqueous interfaces is modulated by interference. C. Luetgebaucks, G. Gonella, **S. Roke**

2:20 ANYL 403. Monitoring photosynthetic metabolism in a microalgal cell by Raman spectroscopy with stable isotope labeling. **Y. Yonamine**, Y. Suzuki, T. Ito, Y. Miura, Y. Ozeki, K. Goda, Y. Hoshino

2:45 ANYL 404. Study of tryptophan analogues as mechanistic probes of indoleamine 2, 3-dioxygenase reactivity. **A.C. Terentis**, T.C. Foo, J. Meacham, S.R. Thomas

3:10 Intermission.

3:30 ANYL 405. Single-molecule tracking studies of charge-dependent translational and orientational dye motions within surfactant- and solvent-filled silica mesopores. **R. Kumarasinghe**, T. Ito, D.A. Higgins

3:55 ANYL 406. DNA hybridization kinetics through analysis of single-molecule binding-time intervals. **E.M. Peterson**, W. Li, M.W. Manhart, J.M. Harris

4:20 ANYL 407. Probing the local dielectric properties of plasmid DNA in solution and adsorbed on chemically graded surfaces. **Z. Li**, R. Kumarasinghe, M.M. Collinson, D.A. Higgins

Section C

Ernest N. Morial Convention Center Room 229 Ambient Ionization & Forensic Science

A. Hall, *Organizer*
B. Musselman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ANYL 408. Development of DART-MS libraries and a reverse library search program for on-site or laboratory screening of seized drugs. **B. Musselman**, F. Li, J. Tice, S. Shrader

2:00 ANYL 409. Direct analysis in real time: A new technique for the forensic paint examiner. **C. Bridge**, M. Maric, R.B. Cody

2:30 ANYL 410. Forensic applications of direct analysis in real time (DART) coupled to mass spectrometry. **J. Almirall**

3:00 Intermission.

3:20 ANYL 411. Detection of falsified medicines via triboelectric nanogenerator (TENG) mass spectrometry. **F.M. Fernandez**, M. Bernier, A. Li, L. Winalski, Y. Zi, Z.L. Wang

3:50 ANYL 412. Characterizing a portable MS system featuring interchangeable, ambient ionization sources for routine forensic evidence screening. **C.C. Mulligan**, W. Fatigante, S. Mukta, A. Stelmack, Z.E. Lawton, K. Evans-Nguyen

4:20 ANYL 413. Degradation of sexual lubricant from vaginal bacterial exposure. **D. Green**, M.J. Beazley, C. Bridge

4:40 Concluding Remarks.

Section D
Ernest N. Morial Convention Center Room 227

Forced Degradations in Pharmaceutical Industry

H. Yarabe, *Organizer, Presiding*

1:30 ANYL 414. Forced degradation case studies in pharmaceutical product development and communication strategies to global health authorities. **T. Graul**

2:00 ANYL 415. Evaluation of relative response factors using small scale fraction collection in forced degradation studies. **P. Hong**, P.R. McConville

2:30 Intermission.

2:45 ANYL 416. Force degradation: Breaking up is never an easy thing. **L. Chimilio**

3:15 ANYL 417. Forced degradation studies for well characterized biologics products. **N. Subbarap**

3:45 ANYL 418. Drug degradation mechanisms: Are they important? **S.W. Baertschi**

Section E
Ernest N. Morial Convention Center Room 226

Target-Responsive Fluorescent Probes for Detection & Diagnosis

R.L. McCarley, *Organizer, Presiding*
H. Ai, *Presiding*

1:30 Introductory Remarks.

1:35 ANYL 419. Activity-based sensing as general design principle for fluorescent probe development. **C.J. Chang**

2:00 ANYL 420. Fluorescent and bioluminescent biosensors for biological signaling. **H. Ai**

2:25 ANYL 421. A far-red emitting fluorescent probe for cytosolic Ca^{2+} ion based on phospha-fluorescein scaffold. **H. Ogasawara**, M. Taki, Y. Sato, S. Yamaguchi

2:50 ANYL 422. Switchable molecular fluorescent probes for detection and imaging of enzymes linked to disease. **R.L. McCarley**

3:15 Intermission.

3:30 ANYL 423. Visualizing intercellular tensile forces by DNA-based membrane molecular probes. **B. Zhao**, M. You

3:55 ANYL 424. Live cell surface conjugation methods for imaging and sensing. J. Majumder, **G. Chopra**

4:20 ANYL 425. Rapid detection of anthrax biomarker based on recovered fluorescence of carbon dots-Cu(II) system. **S.F. Li**

4:45 ANYL 426. Graphene oxide protease sensor for early detection of HIV. **Y. Zhang**, X. Chen, G. M Roozbahani, X. Guan

Inaugural Joint Symposium of the Separation Science Subdivisions
Sponsored by I&EC, Cosponsored by ANYL

Inaugural Joint Symposium of the Separation Science Subdivisions
Sponsored by I&EC, Cosponsored by ANYL

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center Room 228

Monitoring Pharmaceuticals & Other Pollutants in Water
Cosponsored by MPPG‡
S. Ahuja, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 ANYL 427. Monitoring pharmaceuticals and personal care products in water. **S. Ahuja**

9:10 ANYL 428. Pharmaceuticals in the environment and water quality: The role of analytical chemistry. **H. Yao**

9:40 ANYL 429. Novel sample prep platform for monitoring pharmaceuticals and personal care products in water. **C.A. Pohl**

10:10 Intermission.

10:30 ANYL 430. Rapid and sensitive method for the determination of 1,4-dioxane analysis in a wide range of aqueous matrices. **D. Knappe**, M. Sun, C. Lopez

11:00 ANYL 431. Pesticide monitoring using passive sampling for in ground water from Sais, Morocco. **I. Berni**, A. Menouni, I. El Ghazi, R. Duca, L. Godderis, S. El JAAFARI

Section B
Ernest N. Morial Convention Center Room 230

Advances in Spectroscopy

J.M. Harris, *Organizer*
D. Zhang, *Presiding*

8:30 ANYL 432. Using inductively coupled plasma atomic spectroscopy and solid-state NMR spectroscopy to increase characterization speed of polymorphic drugs. **G. Behnke**, R. Quinones, R. Iuliucci

8:55 ANYL 433. NMR solution phase structural determination of antibiotics and comparisons of their predicted docking energies. F. Mahmoudi, **W. Carroll**

9:20 ANYL 434. Measuring the electromagnetic properties of pigments during exposure to ultraviolet radiation. **S. Partridge**, D. Slocombe, J. Bauer, A. Porch

9:45 ANYL 435. Polarized resonance synchronous spectroscopy for nanomaterial characterizations. **D. Zhang**

10:10 ANYL 436. Quantification of the effect of molecular aggregation on fluorophore photon extinction, absorption, scattering, Stokes-shifted fluorescence, and on-resonance fluorescence. **B.C. Nugaduwa Vithanage**, D. Zhang

10:35 ANYL 437. Simplification of the data analysis in polarized resonance synchronous spectroscopy by experimental quantification of instrument response function. **J. Xu**, J. Hu, D. Zhang

11:00 ANYL 438. In-situ UV-vis and PRS2 monitoring gold nanoparticle structure and optical activity variations induced cyanide dissolution. **N.S. Abeynayake**, D. Zhang

Section C
Ernest N. Morial Convention Center Room 229

Advances in Mass Spectrometry

M.F. Bush, *Organizer, Presiding*

8:30 ANYL 439. Effects of drift gas selection on the ion mobility of biomolecular ions, large and small. **M.F. Bush**

8:55 ANYL 440. MultiCRAFTI: Overcoming the kinetic energy limitation to measure the cross section of high-mass ions. **B. Pope**, D. Joaquin, J. Hickey, D.V. Dearden

9:20 ANYL 441. Nanoparticle co-matrix for multiply charged ions in MALDI imaging. **B. Banstola**, K.K. Murray, M. Hossen

9:45 ANYL 442. Fast isotope ratio mass spectrometry (FIRMS): A tandem mass spectrometry technique for the rapid and semi-comprehensive evaluation of isotope ratios. **F. Ochieng**, B.A. Logue, P. Hinker

10:10 Intermission.

10:30 ANYL 443. Characterization of metabolic syndrome related lipids acquired using a novel scanning quadrupole DIA acquisition method. **R.S. Plumb**

10:55 ANYL 444. LC-MS detection of pyrrolizidine alkaloids and their *N*-oxides in herbarium specimens dating back to 1840. **J. Tasca**, C. Smith, E.A. Burzynski, B. Sundberg, A.F. Lagalante, T. Livshultz,

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K.P. Minbiole

11:20 ANYL 445. Testing for rye-phytochemicals in prostate tissue, plasma, and urine from prostate cancer patients. **S.K. Krogh Steffensen**, I.S. Fomsgaard

11:45 ANYL 446. Live single cell mass spectrometry: Towards quantitative analysis. N. Pan, S. Standke, N.R. Kothapalli, A. Burgett, **Z. Yang**

Advances in Bacterial (Nano) Cellulose Research

Bacterial (Nano)Cellulose Formation, Structure & Medical Applications

Sponsored by CELL, Cosponsored by ANYL

THURSDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 228

Advances in Electrochemistry

L.A. Baker, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ANYL 447. Optimization of a 24/7 electrochemical sensor for continuous, on-site analysis of arsenic in water. **K.L. Kaht**, M.M. Crain, T.J. Roussel, R.S. Keynton, R.P. Baldwin

1:55 ANYL 448. Electrochemical, aptamer-based (E-AB) sensors interfaced with three-dimensional (3D) tissue culture to study the role of adenosine triphosphate (ATP) in astrocyte cells. **M. Santos Cancel**

2:15 ANYL 449. Electrochemical sensing with a suspended single nanowire in a microfluidic channel. **R.C. Chiechi**, P. Oomen, Y. Zhang, E. Verpoorte, K. Mathwig

2:35 ANYL 450. Point-of-care determining acetaminophen with multi hydrogen bonds manipulated single-molecule recognization. **Z. Huang**, Y. Zhang, T.E. Wiese, G. Wang, K.E. Riley, Z. Wang

2:55 ANYL 451. Electrochemical monitoring of individual *E. coli* and *B. subtilis* bacteria using electrochemical collisions. **S.N. Thorgaard**, A.T. Ronspees

3:15 Intermission.

3:35 ANYL 452. In situ electrodeposition of RGO for detection of trace metals. **H. Shamkhalichenar**, J. Choi

3:55 ANYL 453. Development of an all-solid-state Fe(II) ion-selective electrode. **T. Ozer**, T. Borch

4:15 ANYL 454. Novel catalyst assessment for CO_2 reduction efficiency. **E. Goel**

4:35 ANYL 455. Development of boron doped diamond paste electrodes for microfluidic paper-based analytical devices. **S. Nantaphol**, R.B. Channon, T. Kondo, W. Siangproh, O. Chailapakul, C. Henry

4:55 ANYL 456. Solid electrolyte interphase and nitrogen doping effect on potassium storage mechanism in graphite. **H. Wang**, J. Liu, P. Liang, Z. Shen

Section B
Ernest N. Morial Convention Center
Room 230

Advances in Spectroscopy

J.M. Harris, *Organizer*
E.M. Peterson, *Presiding*

1:30 ANYL 457. Scattering-type scanning near-field optical microscopy (s-SNOM) and nanoscale spectroscopy (nano-FTIR) on polymers, biomaterials and 2D materials. **P. Schäfer**, T. Gokus

1:55 ANYL 458. Withdrawn

2:20 ANYL 459. FTIR microspectroscopy imaging as a tool to study chemical composition in intact wild type and mutant *C. elegans* strains. **A. Bouyanfif**, S.P. Liyanage, J. Hewitt, S. Vanapalli, N. Moustaid-Moussa, E. Hequet, N. Abidi

2:45 ANYL 460. Computational and spectroscopic studies of pH (Low) insertion peptides in lipid membranes. **J. Flanagan**, C.R. Baiz

3:10 Intermission.

3:30 ANYL 461. pH-dependent surface-enhanced Raman scattering response of silver-loaded microgel particles. T. Curtis, A. King, C. Swanson, **S.R. Emory**, D.A. Rider

3:55 ANYL 462. A silver coated gold nanorod decorated fibrous SERS substrate for arsenic detection. **S. Xu**, B. Chase, D.L. Sparks, J.F. Rabolt

4:20 ANYL 463. Improved chemical identifications by Raman spectroscopy through sequential multimodal powder-, solution-, drop-drying, and surface-enhance- Raman spectral acquisitions. **P.C. Khanal**, J. Xu, J. Hu, D. Zhang

4:45 ANYL 464. Withdrawn

Advances in Bacterial (Nano) Cellulose Research

Pharmaceutical, Medical & Technical Applications

Sponsored by CELL, Cosponsored by ANYL

BIOT

Division of Biochemical Technology

M. Antoniewicz and N. Tugcu, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Biobased Water Purification System Approaches (see *CELL*, Tue)

WCC Rising Star Award Symposium (see *WCC*, Tue)

SOCIAL EVENTS:

Membership Desk, 8:00 AM: Sun, Mon, Tue, Wed, Thu

Reception, 6:30 PM: Sun

Program Chair's Lunch, 12:30 PM: Wed

Company Lunch Seminars, 12:30 PM: Sun, Mon, Tue, Wed, Thu

Networking/Mentoring Session, 6:00 PM: Mon

BUSINESS MEETINGS:

BIOT Executive Committee Meeting, 7:00 PM: Mon

Future Programming Meeting, 12:30 PM: Tue

SUNDAY MORNING

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Automated, High throughput & In Silico Technologies for DSP Development

L.W. Pampel, N. Sanaie, D.W. Wood, *Organizers*
J. Griesbach, J. Hubbuch, S. Parimal, *Presiding*

8:30 BIOT 1. In silico design of integrated downstream processes for non-mAb biologics produced in complex expression systems. **N. Vecchiarello**, C. Goodwine, S.M. Cramer

8:50 BIOT 2. Streamlining early DSP development through evolving integrated mechanistic models. **A.T. Hanke**, R. Khalaf, L.W. Pampel

9:10 BIOT 3. Using a Bayesian framework to account for scale-down model offsets during process characterization. **M. Stork**, A. Cheng, B. Evans, P. Slade, E. Yu

9:30 BIOT 4. Mechanistic modeling analysis of chromatography scale-down models. **S. Benner**, J. Welsh, M. Rauscher, J. Pollard

9:50 Intermission.

10:10 BIOT 5. In-silico model formulation, calibration and application for commercial CEX chromatography. **C. Kunert**, F. Schlegel, K. Westerberg, O. Kaltenbrunner, P. Rolandi, X. Zhu

10:30 BIOT 6. A scale-down methodology using mini-columns to predict chromatography performance in development and production scale columns. **S.T. Evans**, M. Nagarajan, T. Lew, C. Lupis, G. Ferreira, G. Miro-Quesada, D. Robbins

10:50 BIOT 7. Model-based quality by design: Challenges, pitfalls and best practices. **T. Huuk**, M. Casals-Peralvarez, T. Hahn, T.C. Beck, J. Hubbuch

11:10 BIOT 8. Artificial intelligence in protein chromatography: Root cause investigation of process deviations. **G. Wang**, T. Briskot, T. Hahn, P. Baumann, J. Hubbuch

Section A
InterContinental New Orleans
La Salle A

BIOT Awards

David Perlman Memorial Lectureship

M.R. Antoniewicz, N. Tugcu, *Organizers*
T.M. Przybycien, *Organizer, Presiding*

11:30 Introductory Remarks.

11:40 BIOT 9. Designing biology for health and the environment. **P. Silver**

Section B
InterContinental New Orleans
La Salle B/C

End-to-End Biomanufacturing

Process Analysis & Control of Product Quality Attributes

S.W. Harcum, V. Natarajan, N. Rathore, S.A. Tobler, *Organizers*
G. Hiller, C. Jiang, P. Tessier, *Presiding*

8:30 BIOT 10. Process analytical technology for flow synthesis of antisense oligonucleotides: Real-time starting material assurance and ASO sequence confirmation. **X. Su**, J. Yang, A. Ng, E. Schmitt, J. Stolee

8:50 BIOT 11. Paving the road towards real-time release testing. **G. Malmquist**

9:10 BIOT 12. Integrating metabolomics and process analytical technology (PAT) for rapid monitoring of protein glycosylation in a CHO bioprocess. **E. Kamaloo**, E. Hodgman, A. Lewis, J. West, D. Mohammed, B. Drew, N. Aranibar, B.M. Warrack, M.D. Reily, E. Garr

9:30 BIOT 13. Late-phase process improvement: Methods to increase titer while maintaining product quality. **M. Bennett**, M. Zustiak

9:50 Intermission.

10:10 BIOT 14. Differential expression and activity of metabolic enzymes in cell culture fluid correlates with increased disulfide reduction of mAb products. **A.J. Cura**, S. Chollangi, K. McWade, J. Yee, M. Peck, T. Hageman, Y. Huang, X. Xu, S. Ghose

10:30 BIOT 15. Steering N-glycosylation of recombinant proteins using systems engineering. **M.G. McCann**, T.S. Le, C. Stach, X. Chen, N. Somia, L. Zhao, M. Smanski, W. Hu

10:50 BIOT 16. An E2E approach for controlling aggregation through a monoclonal antibody (mAb) process. **S. Saluja**, G. Evangelist, C. Xu, R. Raju, C. Kwiatowski

11:10 BIOT 17. Monitoring and control of capture steps by spectroscopy combined with PLS modeling. **L. Rolinger**, M. Rudt, N. Brestrich, J. Hubbuch

Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Protein Structure & Function

E. Sahin, P.M. Tessier, *Organizers*
X. Ge, R. Shah, *Presiding*

8:30 BIOT 18. Rapid mapping of glycoprotein structure-activity relationships by shotgun scanning glycomutagenesis. **X. Zheng**, M.P. DeLisa

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8:50 BIOT 19. High-throughput single molecule FRET for protein structure-dynamics-function screening and molecular evolution. **K. Hamadani**

9:10 BIOT 20. A novel widespread toxin-antitoxin module. F. Piscotta, **A. Link**

9:30 BIOT 21. Cholesterol dependent ligand binding and downstream signaling of the adenosine A_{2a} receptor. **C. McGraw**, A.S. Robinson

9:50 Intermission.

10:10 BIOT 22. Comparing apples and oranges: Identifying initiator peptides of non-amyloid prions. **C. Jakobson**, J. Byers, T. Lozanoski, Z. Harvey, R. Futia, S. Sahai, M. Swift, D.F. Jarosz

10:30 BIOT 23. Deciphering structural and chemical determinants of pathological tau conformation using yeast surface display. S. Wang, **Y. Cho**

10:50 BIOT 24. Interactions of arginine. HCl and NaCl with protein surfaces: Effect on self-association, aggregation, and viscosity of mAb formulations. **C. Sudrik**, T. Cloutier, P. Pham, H. Samra, B.L. Trout

11:10 BIOT 25. Vibrational Stark effect spectroscopy as a tool for enhancing understanding of electrostatics in complex protein systems. **E.T. Novelli**, L.J. Webb

Section D
InterContinental New Orleans
Frenchman Ballroom

Upstream Processes

Systems Biology & Omics Applications

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
C. Chen, C. Metallo, *Presiding*

8:30 BIOT 26. Investigating the global landscape of chromatin accessibility to improve production Chinese hamster ovary (CHO) cell line stability. **Z. Lee**, W. Hu

8:50 BIOT 27. Advancing mammalian metabolic engineering through kinetic model optimization. **C.M. O'Brien**, A. Allman, P. Daoutidis, W. Hu

9:10 BIOT 28. Leveraging –omics techniques to enhance productivity of biologics in microbes. **J.R. Brady**, C.A. Whittaker, M. Tan, N. Colant, N. Dalvie, K. Love, J.C. Love

9:30 BIOT 29. Mapping the energy profile of cell culture through advanced lipidomics and metabolomics. **A.S. Ali**, A. Gilbert, L. Zang, R. Raju

9:50 Intermission.

10:10 BIOT 30. Interrogation of critical metabolic pathways important for compartment-specific redox homeostasis in cancer cells. **M. Badur**, D. Zhao, J. Luebeck, J. Magana, A. Birmingham, R. Sasik, T. Ideker, C. Metallo, P. Mali

10:30 BIOT 31. From genotype to fluxome to a comprehensive kinetic model of *Escherichia coli*. **M.R. Antoniewicz**

10:50 BIOT 32. Genomic scale metabolic network reconstruction of *Nostoc sp.* PCC 7120 for the analysis of cyanophycin production. **D. Norena-Caro**, M.G. Benton

11:10 BIOT 33. Quantitative multi-dimensional single-cell analysis of autophagy during myogenesis. **H. Brown**, E.A. Arriaga

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

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SUNDAY AFTERNOON

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Emerging Technologies for Downstream Processing of Bionanoparticles

L.W. Pampel, N. Sanaie, D.W. Wood, *Organizers*
M. Bakhshayeshi, S. Kumar, T. Linden, *Presiding*

2:00 BIOT 34. Use of polyamines for enhanced retention of plasmid DNA isoforms during ultrafiltration. Y. Li, **I. Manzano**, A.L. Zydney

2:20 BIOT 35. Scalable nanofiber based lentiviral vector purification. J. Ruscic, C. Perry, Y. Takeuchi, T. Mukhopadhyay, **D.G. Bracewell**

2:40 BIOT 36. mRNA vaccines and therapeutics: On the progress from promise to reality. **H. Pujar**

3:20 Intermission.

3:40 BIOT 37. Virus purification in aqueous two-phase system at varying tie line lengths. **C. Heldt**, P. Joshi, M. Weiss

4:00 BIOT 38. Development of a scalable chromatography process to separate empty and full adeno-associated vector (AAV) particles. **R. Dickerson**, M. Bakhshayeshi

4:20 BIOT 39. *In silico* prediction of physicochemical liabilities in Adeno-associated virus capsids. **K. Manibog**, S. Kumar

4:40 BIOT 40. Single-use purification of cell culture-derived virus particles by steric exclusion chromatography. P. Marichal-Gallardo, K. Lothert, T. Grein, U. Reichl, P.M. Czermak, **M.W. Wolff**

Section B
InterContinental New Orleans
La Salle B/C

Upstream Processes

Mammalian Cell Culture & Engineering: Media and Metabolism

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
Y. Cho, N. Jacob, S. Ozturk, A.B. Tolstrup, *Presiding*

2:00 BIOT 41. Withdrawn

2:20 BIOT 42. Media optimization towards a high-titer platform process. **B.Y. Wong**, R. Shawley, M. Gawlitzek, L. Zhang

2:40 BIOT 43. Elucidating amino acid metabolism in CHO cells. **M.R. Antoniewicz**, J. Gonzalez, B. McConnell, H. Naik, V. Dhara, M.J. Betenbaugh

3:20 Intermission.

3:40 BIOT 44. What cells want vs. what cells need: Simplification of chemically defined media for optimal performance. **M. Krajcovic**, Y. Ilin, S. Hutchins, A. Borshchenko, W.S. Ahn, L. Tescione, D. Inlow, C. Lu

4:00 BIOT 45. Media formulation optimization based on multi-scale modeling of heterogeneity in mammalian cell culture process. **S. Galbraith**, H. Liu, S. Yoon

4:20 BIOT 46. Understanding glycosylation variability in CHO cell cultures. **P. Ahyow**, A. Nguyen Dang, K. Mains, M. Mun

4:40 BIOT 47. Understanding the effect of preparation methods on bioavailability of components in a cell culture feed. **M. Berge**, E. Hackner, J. Lee, J. Reier, M. Liang

Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Protein Interactions & Interfaces

E. Sahin, P.M. Tessier, *Organizers*
D.G. Bracewell, H.D. Sikes, W. Weiss, *Presiding*

2:00 BIOT 48. Dynamic and chemically heterogeneous polymer brushes stabilize protein conformation. D.F. Marruecos, H.H. Kim, D.K. Schwartz, **J. Kaar**

2:20 BIOT 49. Mechanistic origin of the combined effect of surfaces and mechanical agitation on protein aggregation. **P. Arosio**

2:40 BIOT 50. Neutron scattering to characterise protein interactions with solid-liquid interfaces in bioprocessing. **M. Papachristodoulou**, D.G. Bracewell, C.J. Roberts, L. Clifton, P. Butler, J. Doutch

3:00 BIOT 51. Adsorption of non-ionic surfactants and proteins on hydrophobic surfaces studied by neutron reflectometry. **Z. Zhang**, S.V. Orski, A.M. Woys, I. Zarraga, N.J. Wagner, Y. Liu

3:20 Intermission.

3:40 BIOT 52. Withdrawn

4:00 BIOT 53. Computational approaches to understand a living/inorganic interface: Engineering bacterial fimbrial tip protein FimH to bind gold surfaces. **M.C. Small**, J. Terrell, D.N. Stratis-Cullum, M. Hurley

4:20 BIOT 54. Short wave radio frequency resonators for transducing protein and cell surface interactions in closed systems. S. Charkhabi, A. Beierle, **N. Reuel**

4:40 BIOT 55. Determining the relationship between T cell activity and affinity of cytomegalovirus-specific TCRs. **C. Stevens**, C. Williams, Z. Frye, J. Jiang, J. Maynard

Section D
InterContinental New Orleans
Frenchman Ballroom

Biomedical & Emerging Technologies

New Tools & Approaches for Cancer Applications

A.M. Kloxin, A. Noyes, J.P. Pieracci, *Organizers*
J.N. Albert, A. Boesch, J. Spangler, *Presiding*

2:00 BIOT 56. Simultaneous determination of drug efficacy in single cells using a multiplexed droplet trapping array. **K. R Bajgiran**, R. Elkhanoufi, M. Vaithiyanathan, J.A. Dorman, A.T. Melvin

2:20 BIOT 57. Small molecule based drug capture materials. **S. Krishnamoorthy**, R.H. Grubbs

2:40 BIOT 58. Electro-responsive poly-graphene medi-patch arm-bands for controlled delivery of STAT-3 inhibitors in anti-stem cell melanoma therapy. **S.K. Misra**, M.S. Khan, P. Mukherjee, D. Pan

3:00 BIOT 59. Precisely targeted photodynamic antitumor therapy by platelet membrane coated nanoparticle. **L. Xu**, F. Gao, F. Fan, L. Yang

3:20 Intermission.

3:40 BIOT 60. Eradicating primary tumor and cancer stem cells with prosthetic antigen receptor modified T-cells. **C.R. Wagner**, J.R. Petersburg

4:00 BIOT 61. Visualization of a cancer-associated enzyme using near-infrared (NIR) off-on and on-on fluorescent probes in vitro and in vivo. **Z. Shen**, R.L. McCarley

4:20 BIOT 62. Programmed accumulation of prodrug-converting enzymes in cancer cells. **T.D. Warren**, M. Ostermeier

4:40 BIOT 63. Tunable, post-translational method for controlling prodrug converting enzymes in cancer cells. **A. Gaynor**, W. Chen

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

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ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY EVENING

Section A
InterContinental New Orleans
La Salle A

BIOT Tank

G. Bolton, M. Lynch, *Organizers*
V. Roy, *Organizer, Presiding*

5:00 Introductory Remarks.

5:15 BIOT 64. Complete snakebite therapy. **C.F. Komives**

5:30 BIOT 65. *Escherichia coli* as production vehicle for high value chemicals, glucaric acid and glucuronic acid. **D. Prather**

5:45 BIOT 66. Next generation biopharmaceutical process development: Stop experimenting. GoSilico. **T. Huuk**, T.C. Beck, T. Hahn, J. Hubbuch

6:00 BIOT 67. Zepteon: On demand antiviral antibody production. **A. Boesch**, G. Bolton, J. Fox, M. Diamond

6:15 Discussion.

MONDAY MORNING

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Advances in Chromatographic Separations

L.W. Pampel, N. Sanaie, D.W. Wood, *Organizers*
S.M. Cramer, J. Neville, D. Robbins, *Presiding*

8:30 BIOT 68. Exploring the mulitmodal anion exchange space: Fundamental investigations and applications. **J. Robinson**, H. Chen, X. He, Y. Xu, M.A. Snyder, S.M. Cramer

8:50 BIOT 69. Evaluation of chromatofocusing and related ion exchange methods as alternatives to protein A chromatography in purification of antibodies. **Y. Liu**, S. Deldari, H. Guo, C.N. Rao, R. Bates, R. Swanson, Z. Li, S. Ghose, D. Frey

9:10 BIOT 70. A new cation exchange resin designed for the removal of monoclonal antibody aggregates using flow-through frontal chromatography. **M. Stone**, K.A. Cotoni, J. Stoner, P. Menstell

9:30 BIOT 71. Releasing chromatography from the past: Integrating a new lattice supported bed and resin design to achieve hyperproductive™ affinity capture. **M. Siwak**, J. Van Alstine

9:50 Intermission.

10:10 BIOT 72. Control of an engineered self-cleaving affinity tag for purification of recombinant proteins by modulating extein residues. **Y. Fan**

10:30 BIOT 73. Robust viral clearance using novel anion exchange technology. **A.M. Voloshin**, N. Stepanova, A. Castro Forero

10:50 BIOT 74. Retooling downstream processing to address or enable an ever-expanding diversity of therapeutic modalities. **C. Haynes**, D.J. Roush, M.A. Snyder

Section A
InterContinental New Orleans
La Salle A

BIOT Awards

Van Lanen Award and Marvin Johnson Award Lecture

M.R. Antoniewicz, N. Tugcu, *Organizers*
T.M. Przybycien, *Organizer, Presiding*

11:30 Introductory Remarks.

11:40 BIOT 75. Synthetic biology: Putting synthesis into biology. **H. Zhao**

Section B
InterContinental New Orleans
La Salle B/C

End-to-End Biomanufacturing

Big Data & Knowledge Management

S.W. Harcum, V. Natarajan, N. Rathore, *Organizers*
S.A. Tobler, *Organizer, Presiding*
M. Boggara, *Presiding*

8:30 BIOT 76. Application of big data to inform prior knowledge and facilitate process validation risk assessment. **S. Wong**, K. Kaleas, A. White, K. Lazzareschi, J. Persson

8:50 BIOT 77. Leveraging prior knowledge to streamline risk assessment tools and process validation study design. **A. White**

9:10 BIOT 78. Model evolution: Enabling process knowledge continuum and control. **J. Ren**, S. Romero-Torres, C. Shi, R. Guenard

9:30 BIOT 79. Unlocking the potential of big data in a biopharmaceutical manufacturing network. **G. Naugle**, P. Stey

9:50 Intermission.

10:10 BIOT 80. Mining process data to improve environmental impact of biomanufacturing. **K. Budzinski**, M. Blewis, P. Dahlin, J. Esparza, J. Gavin, S.V. Ho, C. Hutchens, D. Kahn, S.G. Koenig, R. Kottmeier, J. Millard, M. Snyder, B. Stanard, L. Sun

10:30 BIOT 81. Application of process data analytics to improve commercial scale mAb manufacturing process. **L. Xu**

10:50 BIOT 82. Application of novel multivariate data analysis (MVDA) techniques to understand and troubleshoot variability in cell culture manufacturing. **L. Cella**, J.S. Bowers, P. Avalle, L. Obando, A. Abdelsalam, K. Thirupapliyur, D. Bonnano, J. Easson, S. Gough, R. Leighty, V. Janakiraman, A. Russo, A.G. Tulloch, G. Maheshwari

11:10 BIOT 83. Understanding upstream variability and new data techniques. **V. Saucedo**

Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Protein Engineering & Design

E. Sahin, P.M. Tessier, *Organizers*
Y. Cho, M. Geddie, *Presiding*

8:30 BIOT 84. MLProScape: Machine learning guided approach for engineering enzymes faster. **S.T. Gupta**, E. Glasgow, B.G. Fox, P. Ramanathan, J. Reed

8:50 BIOT 85. Surface display-enabled selection of bioorthogonally stabilized alpha helices using non-natural amino acid incorporation. **T.A. Navaratna**, L. Atangcho, A. Min, G.M. Thurber

9:10 BIOT 86. Three ways to design selective peptide inhibitors of anti-apoptotic Bfl-1. **A.E. Keating**

9:50 Intermission.

10:10 BIOT 87. Direct measurement of deubiquitinating enzyme activity in intact cells using a protease-resistant, cell permeable peptide-based reporter. **N. Safabakhsh**, J. Pettigrew, T. Gauthier, A.T. Melvin

10:30 BIOT 88. Proteolytic silencing of diverse mammalian protein targets using a functionally remodeled bacterial E3 ubiquitin ligase. **M.R. Baltz**, E.A. Stephens, M.P. DeLisa

10:50 BIOT 89. Implications of protein sequence variants derived from systematic starvation. **E. Wong**, C. Huang, Z. Zhang

11:10 BIOT 90. Design of protein glycosylation sites by high-throughput expression and characterization of polypeptide glycosyltransferases. **W. Kightlinger**, L. Lin, M. Rosztoczy, M.P. DeLisa, M. Mrksich, M.C. Jewett

Section D
InterContinental New Orleans
Frenchman Ballroom

Upstream Processes

Microbial Communities & Microbiomes

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
C.H. Collins, C. McChalicher, O. Venturelli, *Presiding*

8:30 BIOT 91. Microbiome-virome interactions in bovine rumen: Elucidating metabolic transactions through metabolic modeling. M. Islam, W. Schroeder, S. Fernando, **R. Saha**

8:50 BIOT 92. Evaluation of a cyanobacterial consortium for efficient polysaccharide production. **K. Poorey**, R.W. Davis, O. Killian, C. Talbot, D. Smernoff, R. Mancenelli, E. Sundstrom

9:10 BIOT 93. Engineering modular microbial communities for cellulose utilization and bioproduct synthesis. **K.Z. Kalbarczyk**, M. Koffas, C.H. Collins

9:30 BIOT 94. Sustainable production of industrially relevant biomonomers: A photosynthetic microbial consortia approach. **D.N. Carruthers**, E. Marsh, X. Lin

9:50 Intermission.

10:10 BIOT 95. Polysaccharide chemical structure controls on fermentation by gut microbiota, metabolic outputs, and interspecies interactions. Y. Tuncil, M. Chen, T. Yao, **S. Lindemann**

10:30 BIOT 96. ^{13}C metabolic flux analysis in microbial communities: An integrated multi-scale modeling approach. **M.R. Antoniewicz**

10:50 BIOT 97. Electro-active communities for hydrogen production from biomass streams. **A. Lewis**, A. Borole

11:10 BIOT 98. Metabolic modeling of microbial communities. **S. Chan**, C. Maranas

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

MONDAY AFTERNOON

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Advances in Chromatographic Separations

L.W. Pampel, N. Sanaie, D.W. Wood, *Organizers*
S.M. Cramer, J. Neville, D. Robbins, *Presiding*

2:00 BIOT 99. Investigation into the thermodynamics of mAb: Ligand interactions in MM chromatography. **R.B. Gudhka**, D.J. Roush, S.M. Cramer

2:20 BIOT 100. Mechanistic modeling of multi-modal chromatography: Separation of antibody variants using mixed-mode weak cation exchange resins. F. Wittkopp, F. Seelinger, R. Skudas, M. Schulte, **C. Dr. Frech**

2:40 BIOT 101. Case of the disappearing protein peak: Gradient elution behavior in HIC with U-shaped retention factor curves. **A. Creasy**, J. Lomino, G. Barker, G. Carta

3:00 BIOT 102. Modified batch isotherm determination method for mechanistic model calibration. **T. Hahn**, T.C. Beck, T. Huuk, J. Hubbuch

3:20 Intermission.

3:40 BIOT 103. In-depth evaluation of next generation protein A stationary phases. **T.M. Pabst**, J. Thai, A.K. Hunter

4:00 BIOT 104. PEGylating protein A chromatography media increases selectivity and robustness. J.B. Weinberg, **T.M. Przybycien**

4:20 BIOT 105. Increasing productivity of downstream processes; the advantage of antibody based selectivity in the purification of biologics. **P. Hermans**

4:40 BIOT 106. Eshmuno® P anti-A and

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anti-B: Affinity resins for removal of anti-A and anti-B isoagglutinins. **S. Rahane**, M. Turiano, M. Stone, L. Gottlieb

Section B
InterContinental New Orleans
La Salle B/C

Upstream Processes

Mammalian Cell Culture & Engineering: Application of Innovative Technologies

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
Y. Cho, N. Jacob, S. Ozturk, A.B. Tolstrup, *Presiding*

2:00 BIOT 107. Technical capability of Raman spectroscopy for in-line quantification of antibody product quality. **G. Magill**, B. Chiang, B. Horvath

2:20 BIOT 108. Utilization of computational fluid dynamics (CFD) to guide scale up of cell culture bioreactors. **G. Chaudhary**, T. Wucherpfennig, J. Schaefer, E. Hasenfus, J. Wutz, H. Lin, D. Bock, M. Yu

2:40 BIOT 109. Limitations of subcloning as a tool to characterize homogeneity of a cell population. **N. Tejeda**, H. Barkhordarian, T. Tharmalingam, P. Yam, F. Lu, S. Yaghmour, T.P. Munro, C. Goudar, J. Stevens

3:00 BIOT 110. Assessment of the genomic instability of CHO cells for cell line development. **S. O'Brien**, A. Bandyopadhyay, C.M. O'Brien, W. Hu

3:20 Intermission.

3:40 BIOT 111. Development of high-producing CHO cell lines through target-designed strategy. **D. Chen**

4:00 BIOT 112. Unravelling molecular mechanisms that govern the shift to a lactate consumption metabolic state in CHO cell fed-batch cultures. **M. Jacobs**, P. Geoffroy, T. Kalomeris, C. Harrington, B. Mulukutla

4:20 BIOT 113. Cell characterization using a novel online cell quantitation microscopic technology in comparison with conventional offline methodologies. **J. Sun**, V. Doddi, V. Chang, D. Ogawa, T. Luman, H. Lin

4:40 BIOT 114. RNA-seq data reveals metabolic regulation in Chinese hamster ovary cell culture. **S. Yoon**, S. Sha

Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Protein Engineering & Design

E. Sahin, P.M. Tessier, *Organizers*
Y. Cho, M. Geddie, *Presiding*

2:00 BIOT 115. Engineering modular sensing-actuating membrane fusion machinery from influenza hemagglutinin. M. Valverde, J. Price, M.R. Baltz, J. Lee, **E.T. Boder**

2:20 BIOT 116. Yeast as a platform to study adenosine receptor signaling. **A.R. Jain**, A.S. Robinson, C. McGraw

2:40 BIOT 117. Engineering mucoadhesive silk. **G. Petrou**, R. Jansson, M. Högqvist, M. Hedhammar, T. Crouzier

3:00 BIOT 118. Directed evolution of tissue inhibitor of metalloproteinase-1 (TIMP-1) as a selective inhibitor of matrix metalloproteinase-3 (MMP-3). **M. Raeeszadeh Sarmazdeh**, D. Radisky, E. Radisky

3:20 Intermission.

3:40 BIOT 119. Engineering binding affinity and specificity: Application to antibodies targeting phospho- and acetyl-tau. **D. Li**, L. Wang, X. Yao, Y. Cho

4:00 BIOT 120. Optimizing a monoclonal antibody for manufacturability, stability, and cost. **J. Floyd**, C. Siska, A. Gillespie, M. McClure, Y. Brodsky, J. Shaver, R. Clark, R. Ketchem, B. Kerwin

4:20 BIOT 121. Improved library design and selection methods for identifying antibodies with high specificity and solubility. **A. Desai**, L. Rabia, M. Julian, K. Tiller, S.D. Ludwig, Y. Zhang, P. Tessier

4:40 BIOT 122. Engineering novel glycophenotypes in bacteria for the production of authentically glycosylated therapeutic proteins. **X. Zheng**, M.P. DeLisa

Section D
InterContinental New Orleans
Frenchman Ballroom

Biomedical & Emerging Technologies

Stem Cells & Regenerative Medicine

A.M. Kloxin, A. Noyes, J.P. Pieracci, *Organizers*
Y. Kim, M. Kuczewski, *Presiding*

2:00 BIOT 123. Withdrawn

2:20 BIOT 124. Chemically defined microcarriers for the expansion of mesenchymal stem cells. **J. Krutty**, A. Dias, W.L. Murphy, P. Gopalan

2:40 BIOT 125. Cell therapies and their impact on the future of medicine. **K. Niss**

3:20 Intermission.

3:40 BIOT 126. Histone-targeted gene transfer to stimulate chondrogenic MSC differentiation and bone repair. **M.O. Sullivan**, E. Munsell

4:00 BIOT 127. Enzymatically generated hyaluronic acid hydrogel for cytokine therapy of osteoarthritis. **S. Pérez Rafael**, F. Perrone, E. Ramon, T. Tzanov

4:20 BIOT 128. Decoy TRAIL receptor CD264: A predictor of in vitro regenerative potential for mesenchymal stem cells. **S. Madsen**, K. Russell, A. Tucker, J. Glowacki, B. Bunnell, K. OConnor

4:40 BIOT 129. Labeling neural stem cells using trackable ultrasmall iron oxide nanoparticle for cell transplantation therapy. **J. Park**, Y. Kim, Y. Bao, J. Sherwood

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama

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Undergraduate Research Posters

Biotechnology

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MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix

M.A. Blenner, N. Reuel, *Organizers*

8:00–10:00

196, 202-203, 238, 253, 256-257, 263, 265, 269-270, 280, 290, 302, 307, 324, 340, 366, 373-374, 387, 389, 391, 393, 409, 421, 423, 425, 432, 441. See subsequent listings.

TUESDAY MORNING

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Advances in Chromatographic Separations

L.W. Pampel, N. Sanaie, D.W. Wood, *Organizers*
S.M. Cramer, J. Neville, D. Robbins, *Presiding*

8:30 BIOT 130. Chromatography modeling in purification development: Assessing accuracy of predictions to select phase-appropriate modeling strategies. **F. Stueckler**, K. Doninger, J. Yang, C. Williams, T. Briskot

8:50 BIOT 131. Withdrawn

9:10 BIOT 132. Development of an overload chromatography step for high titer processes. **X. Lin**, A. Seay, C. Williams

9:30 BIOT 133. Two column mAb purification platform: Evaluation of AEX step for aggregate clearance. **A. Shirke**, D. Kanani, M. Jin

9:50 Intermission.

10:10 BIOT 134. Downstream process control of aggregates using light scattering and real time molecular weight. **A. Gospodarek**, B. Patel, M. Larkin, S. Kendrick, M. Brower, D.D. Richardson, N. Tugcu

10:30 BIOT 135. In-line Fourier-transform infrared spectroscopy as a versatile process analytical technology for preparative protein chromatography. **A. Sanden**, S. Grosshans, M. Rudt, N. Brestrich, J. Morgenstern, S. Heissler, J. Hubbuch

10:50 BIOT 136. Two-peak elution behavior of therapeutic IgG4 on cation exchange chromatography. **Z. Chen**, M. Wang, X. Xu, S. Ghose

11:10 BIOT 137. Impact of process parameters on a double-peak elution profile of a mAb during CEX chromatography. **L. Konher**, V. Manickam, M. Sharma, B. To, M. Zhu

Section A
InterContinental New Orleans
La Salle A

BIOT Awards

W.H. Peterson Awards & BIOT Young Investigator Award

M.R. Antoniewicz, N. Tugcu, *Organizers*
T.M. Przybycien, *Organizer, Presiding*

11:30 Introductory Remarks.

11:40 BIOT 138. Metabolic engineering strategies for producing oleochemicals in bacteria. **B. Pfleger**

Section B
InterContinental New Orleans
La Salle B/C

End-to-End Biomanufacturing

Challenges in Tech Transfer

S.W. Harcum, V. Natarajan, N. Rathore, S.A. Tobler, *Organizers*
J. Erickson, P. Lewus, *Presiding*

8:30 BIOT 139. MAT & EMBER: CFD modeling framework for optimizing mixing and aeration-agitation strategies in mixing tanks and bioreactors. **A. Munir**, J. Fisher, G.T. Frank, T. Kellogg, P. Rolandi

8:50 BIOT 140. Introduction of a flexible 2000L single-use bioreactor platform: Technology transfer and process-fit challenges in downstream processing. P.R. Smith, J.E. Crawford, D.N. Paolella, **A.R. Ubiera**

9:10 BIOT 141. Maintaining product quality across multiple site-to-site transfers for a commercial mAb: Some successes and lessons learned. **S.A. Tobler**, A.G. Tulloch

9:30 BIOT 142. Tech transfer: The challenges and opportunities represented by a rapidly evolving product pipeline and global manufacturing network. **P. Gammell**

9:50 Intermission.

10:10 BIOT 143. Challenges overcome and robustness improvements in technology transfer of formulation and filling of a vaccine pre-filled syringe. **R.P. Kasprow**

10:30 BIOT 144. Application of small-scale modeling to de-risk filling processes of drug product formulations. **D.M. Saldana**, S. Hanslip, P. Chaffin, M. Palmer, A. Gidh, I. Rusanov, R. Forcino, M. Dimps, K. Desai, I. Kemp

10:50 BIOT 145. Driving change in biomanufacturing through innovation in processes, technologies and operations.

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E. Clark

Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Protein Conjugates & Materials

E. Sahin, P.M. Tessier, *Organizers*
B. Demirdirek, G.M. Thurber, *Presiding*

8:30 BIOT 146. Polymer conjugation to enhance cellulase activity and preserve thermal and functional stability. **T.A. Wright**, M. Lucius, B. Schmitz, K. Burridge, K. Makaroff, J. Stewart, H. Fischesser, J. Shepherd, J. Berberich, D. Konkolewicz, R.C. Page

8:50 BIOT 147. Care packages: Developing a cell-free glycoprotein synthesis platform for portable, on-demand antibacterial vaccine production. **J.C. Stark**, T. Jaroentomeechai, M. Li, R.S. Dubner, K.J. Hsu, T.C. Stevenson, M.P. DeLisa, M.C. Jewett

9:10 BIOT 148. Targeting glyco-immune checkpoints for cancer immune therapy. **C.R. Bertozzi**

9:50 Intermission.

10:10 BIOT 149. Enzymatic construction of EpCAM targeting delivery systems by protein farnesyltransferase. **Y. Zhang**, F. Xu, J. Schaefer, A. Plückthun, M.D. Distefano

10:30 BIOT 150. Engineering a blue light inducible SpyCatcher system (BLISS) for *in vitro* photo-pattering of proteins and optically controlled protein rescue. **E. Hartzell**, J. Terr, W. Chen

10:50 BIOT 151. Enhancing the chemical versatility of yeast display to discover potent, specific enzyme inhibitors. J.T. Stieglitz, H.P. Kehoe, L. Quinto, G. Berumen, J.B. Lissoos, **J.A. Van Deventer**

11:10 BIOT 152. Engineered binding proteins as replacements for antibodies in immunoassays. **H.D. Sikes**, E.A. Miller, K. Sung

Section D
InterContinental New Orleans
Frenchman Ballroom

Upstream Processes

Microbial Metabolic Engineering

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
Z. Rui, R. Sillers, K. Solomon, A. Van Maris, *Presiding*

8:30 BIOT 153. Optimization of heterologous mevalonate production in *E. coli* with a combinatorial promoter library and novel biosensor. **J. Englaender**, A.W. Murfee, K. Solomon

8:50 BIOT 154. Exploring non-natural pathways and native efflux systems for improved aromatic chemical production in *Escherichia coli*. **M. Machas**, G. Kurgan, X. Wang, D. Nielsen

9:10 BIOT 155. Building a bridge between cell-free experimentation and cellular metabolic engineering. **A. Karim**, Q. Dudley, A. Juminaga, S. Crowe, J. Heggestad, W. Grubbe, Y. Yuan, R. Jensen, S. Simpson, M. Koepke, M.C. Jewett

9:30 BIOT 156. Use of an *Escherichia coli* pyruvate-overproducing platform strain to produce L-valine. **P.A. Adamczyk**, S. Pan, X. Zhang, J. Reed

9:50 Intermission.

10:10 BIOT 157. Tailoring chain-length specificity for oleochemical production in bacteria. **N.J. Hernandez Lozada**, B. Pfleger

10:30 BIOT 158. Understanding lipogeneity in oleaginous yeast: source of reducing equivalents for proliferating cell and non-proliferating cell. **P. Xu**

10:50 BIOT 159. Transcriptional-sensor based increase in peroxisomal fatty acyl-CoA flux improves fatty alcohol production in *Yarrowia lipolytica*. M. Shabbir-Hussain, **M. Spagnuolo**, M.A. Blenner

11:10 BIOT 160. Engineering gut fungal membrane-embedded transporters for metabolic engineering in *Saccharomyces cerevisiae*. **I. Podolsky**, S. Seppälä, M.A. O'Malley

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

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TUESDAY AFTERNOON

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Advances in Non-Chromatographic Separations: Harvest Technologies

L.W. Pampel, N. Sanaie, *Organizers*
D.W. Wood, *Organizer, Presiding*
R. Sheth, A.L. Zydney, *Presiding*

2:00 BIOT 161. Guanidine-containing polymers as flocculating agents and filtration aids: Harvest solution alternatives to the centrifuge? **J.K. Rasmussen**, A. Vail, T.D. Bonilla, D.H. Brandwein

2:20 BIOT 162. Clarisolve® mPAA polymer: A stimulus-responsive flocculation polymer for cell culture clarification. **M.J. Susienka**, K.A. Cotoni, J.P. Amara, C. Gillespie

2:40 BIOT 163. Inline flocculation for harvest clarification. **A. Gupta**, J. Castano, E.M. Goodrich

3:00 BIOT 164. Considerations for process development and implementation of fully synthetic depth filters. **D. Ornek**, J. Souther, T. Parker

3:20 Intermission.

3:40 BIOT 165. Aligning acoustic wave separation with concentrated fed batch processing. **M. Collins**

4:00 BIOT 166. Evaluation of gravity settling for disposable harvest. **D. Lok**, E. Chan, E. Mahajan, R. St John

4:20 BIOT 167. Perfusion membrane selection to enable continuous capture chromatography. **R. Piper**

4:40 BIOT 168. Ceramic membrane filtration for biopharms: Potential application for the mammalian harvest process. **A. Ryan**, N. Thite, C. Jung

Section B
InterContinental New Orleans
La Salle B/C

Upstream Processes

Mammalian Cell Culture & Engineering: Novel Modalities and Platforms

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
Y. Cho, N. Jacob, S. Ozturk, A.B. Tolstrup, *Presiding*

2:00 BIOT 169. Overcoming cell line limitation and improving medium in a perfusion process for manufacture of a labile and difficult-to-express enzyme. **J. Lee**, B. Williams, P. Amaya, C. Klaver

2:20 BIOT 170. Maintaining product quality from early to late stage upstream process development. **L. Yung**

2:40 BIOT 171. Improving global access to biotherapeutics. **D. Pettit**

3:20 Intermission.

3:40 BIOT 172. Production and purification of oncolytic measles viruses. T. Grein, H. Dieken, D. Loewe, D. Salzig, T. Weidner, **P.M. Czermak**

4:00 BIOT 173. Impact of high extracellular lactate on induced pluripotent stem cell metabolism. **D. Odenwelder**, S.W. Harcum

4:20 BIOT 174. Investing in process development for MSC production in stirred tank bioreactors. **T. Hood**, J. Ring, T. Lawson, M. Pease, K. Levine, A. Schnitzler, J. Murrell

4:40 BIOT 175. Engineering uniform-shear rate bioreactors to mimic bone marrow and lung vasculature niches for the production of platelets ex vivo. **A. Martinez**, R. McMahon, M. Horner, D. Doser, W.M. Miller

Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Protein Therapeutics

E. Sahin, P.M. Tessier, *Organizers*
E.M. Furst, J. Hubbuch, M. Krause, J.A. Van Deventer, *Presiding*

2:00 BIOT 176. Assessing multi-scale molecular modeling and biased search algorithms for candidate selection with respect to biophysical stability. **C.J. Roberts**

2:20 BIOT 177. Physiochemical determinants of drug-like monoclonal antibodies. **L. Rabia**, S.D. Ludwig, Y. Zhang, M. Julian, P. Tessier

2:40 BIOT 178. Developability of antibodies: Viscosity of high concentration formulations. **R.B. Shah**, E. Carvalho, A.J. Ilott, E. Guo, P. Soler, S. Hart, M. Desai

3:00 BIOT 179. Effects of chemical oxidation on the structure, stability, aggregation, and function of an IgG1 mAb. **D. Shah**

3:20 Intermission.

3:40 BIOT 180. Investigating a correlation between chemical degradation and gelation behavior observed for a monoclonal Fab. **C. Petry**, Y. Zhao, L. Yi, S. Pizarro, A. Wakankar, J. Liu

4:00 BIOT 181. Impact of freezing and thawing rates on protein aggregation for drug substance long term storage. **A. Borwankar**, N. Parsaei, C. Du, N. Singh, S. Ghose, Z. Li

4:20 BIOT 182. High-throughput platform for monitoring protein aggregation kinetics and rapid formulation development. M.F. Drenski, H.P. Rahn, **R.D. Montgomery**

4:40 BIOT 183. PLGA-bevacizumab implants for long-acting anti-VEGF efficacy in a rabbit retinal vascular leakage model. R. Chang, J. Jamison, D.A. Antonetti, **S.P. Schwendeman**

Section D
InterContinental New Orleans
Frenchman Ballroom

End-to-End Biomanufacturing

Automated Technologies & High-Throughput Systems in Biologics Production

S.W. Harcum, V. Natarajan, N. Rathore, S.A. Tobler, *Organizers*
M. Ottens, J. Pollard, *Presiding*

2:00 BIOT 184. Development and validation of a purification platform for proteins expressed in a CHO cell-free system. **S. Deldari**, Y. Liu, H. Guo, C. Gurramkonda, D. Burgenson, S. Borhani, G. Rao, D. Frey

2:20 BIOT 185. Development of a pharmacy-scale, integrated, automated, multi-product platform for on-demand manufacturing of high quality biologics. **L. Crowell**, A. Lu, A. Stockdale, W. Doherty, A. Bonnyman, K. Love, J.C. Love

2:40 BIOT 186. Using HTPD to link AMBR and purification to assess manufacturability of cell line clones. R. Zolyomi, **H. Tjandra**, Y. Chang, A. Hesslein

3:00 BIOT 187. Development of a novel, high-throughput platform for efficient perfusion-based cell culture process development. **T. Gagliardi**

3:20 Intermission.

3:40 BIOT 188. Predicting membrane performance for the concentration and diafiltration of mAb solutions using an ultra scale-down method. **L. Fernandez-Cerezo**, J. Pollard, M. Hoare, A. Rayat, A. Chatel, G. Lye

4:00 BIOT 189. Automated single pass tangential flow filtration (SPTFF) for lab scale continuous bioprocessing. **M. Ghodbane**, N. Thite, C. Jung

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4:20 BIOT 190. Increasing process knowledge using high throughput RoboColumns. **T. Tully**, B. Huffman, M. Stork

4:40 BIOT 191. Innovations in high throughput formulation screening: Promise and reality. **C. Ren**, K. Westland, J. Yeary, M. Boggara, N. Rathore

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

WCC Rising Star Award Symposium
Sponsored by WCC, Cosponsored by BIOT, CHED, COLL, INOR and PROF

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

TUESDAY EVENING

Section A
InterContinental New Orleans
La Salle A

BIOT Awards

3M Poster Award & Industrial Biotechnology Award Lecture

M.R. Antoniewicz, N. Tugcu, *Organizers*
T.M. Przybycien, *Organizer, Presiding*

5:00 Introductory Remarks.

5:10 BIOT 192. How the Janssen-Biogen partnership enabled delivery of a breakthough therapy for multiple myeloma patients and rapid process optimization to meet market demand. **G. Schaefer**

Section B
Ernest N. Morial Convention Center
Hall E

BIOT Poster Session

M.A. Blenner, N. Reuel, *Organizers*

6:00–8:00

BIOT 193. Withdrawn

BIOT 194. Acceleration of native chemical ligation. **S. Jin**, R.J. Brea, N.K. Devaraj

BIOT 195. Nanoparticle mediated release of polymersomes under single pulsed femto second irradiation. **A.R. Robinson**, G.M. Disalvo, S.M. O'Malley, D.M. Bubb, J.C. Griepenburg

BIOT 196. Design and characterization of a benzylguanine-PEG surface for anchoring cellular-derived giant plasma membrane vesicles. **D. Oseid**, A.S. Robinson, J. Albert, S. Lear, A. Cui

BIOT 197. Physical properties of cartilage extracellular matrix. **F. Horkay**, E. Dimitriadis, I. Horkayne-Szakaly, P.J. Basser

BIOT 198. Temporal control of encapsulant release from polymersomes upon single pulse irradiation. **G.M. Disalvo**, A.R. Robinson, J.C. Griepenburg, D.M. Bubb, S.M. O'Malley

BIOT 199. Near infrared responsive polymeric actuator. **I. Hill**, K. Nikolaidou, J. Lu

BIOT 200. Heterochiral DNA circuitry: Interfacing L-DNA with endogenous RNAs. **J.T. Sczepanski**

BIOT 201. Rosmarinic acid particles with versatile biomedical functions. **M. Sahiner**, D.A. Blake, N. Sahiner

BIOT 202. DNA-based nano-constructs for visual detection of rifampin resistant *Mycobacterium tuberculosis*. **R. Connelly**, S. Solarez, Y. Gerasimova

BIOT 203. Creating DNA computer: Five integrated NAND gates with half-adder function. **T. Molden**, M. Grillo, D.M. Kolpashchikov

BIOT 204. Translation of a drug delivery system for glaucoma surgery patients: Challenges in bench-to-bedside design. **M. Fullerton**, B. King, R.S. Ayyala, V.T. John, D.A. Blake

BIOT 205. Expanding the application fields of liquid-handling stations by integrating microfluidics and 3D (bio-) printing. **C. Radtke**, J. Morgenstern, N. Hillebrandt, J. Hubbuch

BIOT 206. Peptoid grafting on polysulfone membrane to increase antifouling characteristics: Effect of grafting density and chain length. **N. Mahmoudi**, J. Moore, M.V. Klaus, G. Harrison, J. Hestekin, **S.L. Servoss**

BIOT 207. Translating unnatural amino acids with computationally-engineered promiscuous EF-Tu variants for broader applications in synthetic polymer synthesis. **V. Cox**, M.F. Matsuura, E.A. Gaucher

BIOT 208. Tanshinone as a dual amyloid Inhibitor against the aggregation and toxicity of both amyloid-β and hIAPP. **B. Ren**, Y. Liu, Y. Zhang, F. Yang, J. Zheng

BIOT 209. Discovering antibody binding signatures in age-related macular degeneration for diagnostic development. **J. Bozekowski**, P. Daugherty

BIOT 210. Development of phage strategies to identify affinity peptide ligands against antibody kappa Fab fragments. **A. Nascimento**, A. Mullerpatan, R. Ghosh, M. Aires-Barros, A. Azevedo, P. Karande, S.M. Cramer

BIOT 211. Monoclonal antibody-derived peptides carrying chemical modifications induce immunogenicity in a transgenic mouse model. **B. Peters**, Y. Wang, A. Iglesias, C. Schoneich

BIOT 212. Recent advances in affinity maturation with the assisted design of antibody and protein therapeutics (ADAPT) platform. **C.R. Corbeil**, T. Sulea, E.O. Purisima

BIOT 213. The effect of a formulation excipient on monoclonal antibody tryptophan oxidation. **J.Y. Yang**, A. Strahan, S. Alavattam, Y. Wang, B. Kabakoff, C. Salisbury

BIOT 214. Bispecific antibody process development and evaluation of critical parameters during Fab arm exchange. **M.J. Sobkow**, **D. Bezila**, **R. Bertrand**, A. Detzel, A. Salehi, K. Van Citters, P.J. Alfonso

BIOT 215. Utilizing minimal-volume analytical techniques to assay the structural heterogeneity of IgG1 during clone selection. **P. Angart**, C. Kohnhorst, B. Kuang, S. Velugula, C. Agarabi

BIOT 216. Rapid aggregate reduction of bi-specific antibody model by filtration. J. Adiletta, **R. Alsop**, C. Breuning, L. Pecore, A. Mak

BIOT 217. Establishing a high-throughput process development platform for an antibody conjugation process. **S. Andris**, M. Wendeler, J. Hubbuch

BIOT 218. Challenges in developing a FRET assay to measure monoclonal antibody aggregates. **Z. Oshinbolu**, R. Shah, G. Finka, M. Molloy, D.G. Bracewell

BIOT 219. Withdrawn

BIOT 220. Serum antibody epitope discovery using pattern tiling. **M. Paull**, P. Daugherty

BIOT 221. Extreme thermophiles as metabolic engineering platforms: Tailoring the process to the product. **C.T. Straub**, B.M. Zeldes, J.M. Conway, J.R. Crosby, J.K. Otten, R.M. Kelly

BIOT 222. Development of an engineered *Escherichia coli* consortium for bioconversion of multi-substrate biomass streams to commodity chemicals and fuels. **F. Liu**, M. Tran-Gyamfi, J. Jaryenneh, X. Zhuang, E. Monroe, R.W. Davis

BIOT 223. Research on remediation the NO_3^-N polluted groundwater by the synergistic effect of autotrophic and heterotrophic denitrification. **M. Lan**

BIOT 224. Programmable DNA-guided artificial restriction enzymes. **B. Enghiad**, H. Zhao

BIOT 225. Spatially organizing biochemistry: Choosing a strategy to translate synthetic biology to the factory. **C. Jakobson**, M. Slininger Lee, D.T. Ercek, N. Mangan

BIOT 226. Portable educational tools for synthetic biology. **J.C. Stark**, A. Huang, T.C. Ferrante, R.S. Dubner, K.J. Hsu, P.Q. Nguyen, N. Donghia, K. Pardee, J. Collins, M.C. Jewett

BIOT 227. Withdrawn

BIOT 228. Marine-derived and cold-adapted recombinant functional tyrosinase, that is functionally available as a monophenol monooxygenase. **E. Kang**, Y. Choi

BIOT 229. Using pH-responsive lignin amphoteric surfactant to recycle cellulase by electrostatic interaction. C. Cai, Q. Xue, **H. Lou**

BIOT 230. Comparison of substrates for colorimetric assays using peroxidase-like deoxyribozyme PW17. **M. Tran**, Y. Gerasimova, R. Connelly

BIOT 231. Investigation into autocatalytic intramolecular isopeptide bond forming reaction sites. **S.P. Kasson**, K. Yoshimatsu

BIOT 232. Site-specific incorporation of the TEMPO organic catalyst into a thermostable alcohol dehydrogenase produces a selective bio/organo- hybrid catalyst. **W. Abdallah**, L. Lancaster, D. Hickey, S.D. Minteer, I.R. Wheeldon, S. Banta

BIOT 233. Increase in expression levels, cell lysis, protein refolding and purification efficiency in recombinant Streptokinase using a non Beta Lactum marker for improved patient safety profile in thrombolysis applications for STEMI patients. **D. Ghosh**

BIOT 234. Designing synthetic metabolons via dCas9-guided assembly. **E.o. Berckman**, W. Chen

BIOT 235. Comparison of transfection methods on yield of recombinant human IgG1 Fc. **E.A. Wells**, A.S. Robinson

BIOT 236. Engineering stable anaerobic consortia by understanding the genomic basis for syntrophic interactions. **J. Brown**, X. Peng, S. Gilmore, J. Henske, M.A. O'Malley

BIOT 237. mRNA volatility as a strategy in designing and implementing effective antisense. C. Endicott, Y. Cho, **R. Srivastava**

BIOT 238. Opportunities for facility-enabled science at the DOE Joint Genome Institute (JGI). **Y. Yoshikuni**

BIOT 239. Improving human A1 adenosine receptor expression in yeast towards applications in therapeutics screening and development. **A.R. Jain**, A.S. Robinson

BIOT 240. Aromatic metabolism of 50 non-model oleaginous yeasts. **A. Yaguchi**, K. Boundy-Mills, M.A. Blenner

BIOT 241. Optimizing amino acids in defined media for *Pichia pastoris* recombinant protein expression. **A. Kuo**, C.B. Matthews, K. Love, J.C. Love

BIOT 242. Evaluation of L-asparaginase production in flask, tray bioreactor and in-house designed rotary bioreactor using isolated *Aspergillus* sp. **K. Doriya**, S.K. Devarai

BIOT 243. High-throughput assessment of a novel, thiol-acrylate hydrogel for tumor spheroid synthesis in a microfluidic device. **N. Kersker**, W. Wortmann, N. Safabakhsh, A.T. Melvin, J.A. Pojman

BIOT 244. dsDNA cleavage via deoxyribozyme DNA construct. **M. O'Steen**, D.M. Kolpashchikov

BIOT 245. Optimization of probiotic *E. coli* Nissle 1917 cell-free protein expression system for rapid testing of novel components. **K. Beabout**, M. Goodson, S. Harbaugh, J.L. Chavez, N. Kelley-Loughnane

BIOT 246. Quantification of the effects of high shear stresses on single circulating tumor cells using a microfluidic device. **G. Landwehr**, A. Kristof, J. Balhoff, J. Pettigrew, S. Rahman, A.T. Melvin

BIOT 247. Best practice considerations for development and implementation of a mammalian cell culture perfusion process. P. McInnis, I. Coleman, D. Rank, E.M. Goodrich, **M.A. Cunningham**

BIOT 248. Transitioning from a daily cell bleed perfusion process to a continuous, automated bleed process using a mAb-

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expressing CHO cell line. **P. McInnis**, D. Rank, M.W. Phillips

BIOT 249. Improvements To CHO cell culture scale-down model across multiple scales. **S. McDermott**, A. Bawn, N. Abu-Absi

BIOT 250. Investigating the link between pCO_2 and protein quality in CHO cell culture. A. Connor, **B. Reed**, A. Lewis, E. Garr

BIOT 251. Culture strategies enhancing the suspension adapted CHO-DXB11-S1 high producing cell line expression. **B. Chen**, H. Lu, D. Chen, W. Chi

BIOT 252. Characterizing CHO cell metabolism in glutamine-limited and supplemented feeds during different stages of exponential growth. **B.J. Kirsch**, S.V. Bennun, A.S. Johnson, S.M. Lawrence, M.J. Betenbaugh

BIOT 253. Integrating high throughput analytics with early-stage cell line development; a comprehensive quality attribute characterization of CHO clone candidates expressing a model IgG1 antibody. **C. Kohnhorst**, P. Angart, **B. Kuang**, S. Velugula, D.N. Powers, C. Agarabi

BIOT 254. Effective CHO lead clone selection for late phase process development in a tight timeline. **C.L. Oliveira**, J. Xu, M. Rdultowki, M. Rehmann, A. Yongky, B. Eagan, M.C. Borys, Z. Li

BIOT 255. Evaluation of growth kinetics and antibody quality in mycoplasma-contaminated CHO cell bioreactor cultures. **E. Berilla**

BIOT 256. Rapid process monitoring & control in mammalian cell culture using off-gas mass spectrometry analysis. **H. Goh**, M. Sulu, G. Lewis, G. Josland, A.K. Velayudhan

BIOT 257. Multiplex characterization of Chinese hamster ovary host cell protein interactions with monoclonal antibodies by yeast surface display. A. Castiel, C. McGovern, **K.M. Doolan**

BIOT 258. Systematic analysis of the effect of trace metal variability on therapeutic protein production in CHO cells. **K. McHugh**, S. Sarnik, A. Deresienski, K. Aron, B. Drew, M.C. Borys, Z. Li

BIOT 259. DOE optimization of titer and quality of IgG titer and quality using high-throughput micro-bioreactor system for CHO cell media and supplements. **S. Velugula**, A. Williams, C. Hsu, N. Trunfio, B. Chavez, C. Agarabi

BIOT 260. Differential responses of CHO cells adapted to limitation of inorganic phosphate, glucose or glutamine. **V. Maralingannavar**, D. Parmar, T. Pant, C. Gadgil, V. Panchagnula, M. Gadgil

BIOT 261. Improved DNA double-strand break repair may reduce production loss in Chinese hamster ovary cells. **X. Zhang**, K. Lee

BIOT 262. The interactive effect of trace elements and chelating agents on mammalian cell culture performance in chemically defined media. **Y. Ilin**, M. Krajcovic, S. Hutchins, A. Borshchenko, L. Tescione, D. Inlow, C. Lu

BIOT 263. From 0.5 g/L to 10 g/L: A collective effort to improve upstream production for a fast-track program. **B.M. Gupta**, L. Hoshan, J. Cacciatore, Z. Du, H. Chen

BIOT 264. Evaluation of perfused high density seed bioreactor step of a legacy biologics process. **D. Harrison**, E. Hodgman, E. Garr

BIOT 265. Considerations for implementation of a virus barrier filter for cell culture media. **D. Bohonak**, S. Bates

BIOT 266. Liver toxicity comparisons of small molecule drugs in a high-throughput 3D *In vitro* culture system and in humanized liver mice. **D. Bruckner**, J.M. Connerney, J.S. Dordick

BIOT 267. Enhanced biopharm manufacturing facility utilization via the use of larger volume and higher cell density bags to initiate seed expansion. **G. Laslo**, D. Bhanushali

BIOT 268. Characterization and identification of protein components in glanded and glandless cottonseeds. **K. Sethumadhavan**, H. Cao

BIOT 269. Increasing culture productivity through alternative nutrient supplementation. **K. Mathur**

BIOT 270. High-throughput single cell screening for expression of recombinant proteins in *Escherichia coli* and *Vibrio natriegens*. J. Eichmann, **T. Weidner**, D. Gerlach, P. Czermak

BIOT 271. Impact of Pluronic® F68 on hollow fiber filter-based perfusion culture performance. **R. Jiang**, Y. Chen, F. Wang, S. Xu, H. Chen

BIOT 272. High throughput screening of deubiquitinating enzyme activity in single intact cells using a cell permeable peptide-based reporter and a microfluidics droplet trapping array. **N. Safabakhsh**, M. Vaithiyanathan, S. Sombolestani, A.T. Melvin

BIOT 273. Continuous in-line virus inactivation for next generation bioprocessing. **M. Holstein**, L. Mullin, K.A. Cotoni, R. Tuccelli, J. Caulmare, L. Messier, C. Gillespie, P. Greenhalgh, M.W. Phillips

BIOT 274. *De novo* small molecule design using deep learning models trained on SMILES strings. **P. Ghatty**

BIOT 275. Implementation of process analytical technologies in commercial manufacturing to realize a biologics drug substance enhanced control strategy. **D.R. Hill**, C. Jiang

BIOT 276. Enhanced perfusion process development utilizing ambr at clone selection. **B. Holman**, K. Lee, J. Lee

BIOT 277. Solvent compatibility and extractables profile for use of Mobius® single-use assemblies in ADC processing. **D. Kinzlmaier**, J. Shea, S. Bell, S. Ryan, E.M. Goodrich

BIOT 278. Implementation of single-use powder delivery systems in continuous bio-manufacturing processes: A case study. **P.S. Vengsarkar**, J. Oh, E. Bolessa, N. Deorkar

BIOT 279. Robust platform cell culture processes utilizing the Selexis expression system for decreasing process development timelines and enhancing speed to clinic. **S. Rameez**, Y. Gowtham, S. Gopalakrishnan, K. Zhang, S.S. Mostafa, A.A. Shukla

BIOT 280. Case study: Virus risk mitigation in cell culture media lab-scale to pilot-scale – virus retentive filtration and cell growth studies. **S. Dolan**, B. Wong, R. Alsop, B. Kanoh, B. Hansmann, R.D. Kiss

BIOT 281. High seed density cell culture processes to reduce manufacturing cycle times. **Y. Gowtham**, S. Rameez, S. Gopalakrishnan, K. Zhang, S.S. Mostafa, A.A. Shukla

BIOT 282. Versatility of the continuous chromatography platform. **C. Sun**, R. Quesenberry

BIOT 283. Development of a fully automated high-throughput (HT) method to screen cleaning conditions during a resin lifetime study. **K. Larson**, A. Rodriguez, M. Aswath, A. Naresh, M. Zhu

BIOT 284. Advances in affinity purification technologies for monoclonal antibody capture. **K. Mehta**, A. Venkatesh, P. Shah, G. Bolton, R.G. Soderquist

BIOT 285. Withdrawn

BIOT 286. Withdrawn

BIOT 287. Withdrawn

BIOT 288. High-resolution separation of monoclonal antibody charge variants using a cuboid packed-bed device. **G. Chen**, A. Gerrior, R. Ghosh

BIOT 289. Development of a chromatography-based hydrophobicity assay for viral particles. **A.H. Schwartz**, A.A. Walsh, C. Romanowski, M.S. Burnham

BIOT 290. Use of high-throughput process development (HTPD) methods to develop a toxicology process: Cation and anion-exchange chromatography development case study. **A. Bill**

BIOT 291. Effect of sporicidal sanitization with oxidizing agent on protein A resins: Lifetime and purification performance. **A. Graanberg**, E. Monie, T. Bjorkman, M. Wetterhall, S. Musunuri, K. Oberg

BIOT 292. Increased lifetime of RPC resins in insulin production by clean-up using WorkBeads 40S. **A. Heijbel**

BIOT 293. Development and evaluation of a novel high capacity protein A chromatography resin with significantly increased alkaline stability. **A. Forss**, T. Bjorkman, J. Vasic, M. Ander

BIOT 294. Mixed-mode resin screening for isolation of recombinant thioredoxin from *E. coli*. **A. Ravi**, S. Guo, Z.L. Nikolov, P. Heifetz

BIOT 295. Acidic IgM purification using anion exchange and mixed mode chromatography. J. Greenwood II, **C. Voss**, **W. Rushton**, P. Khandelwal

BIOT 296. Distribution of a unique process derived charged monoclonal antibody species across a cation exchange column. **C. O'Brien**, A. Grecco, L. Gonzalez, I. Alickolli, H. Malanson, J. Pike, S. Sui

BIOT 297. Implementation of multi-column chromatography for affinity purificaiton. **C. Snyder**

BIOT 298. Capacity and beyond: Evaluation of a next generation protein A resin. **C. Furcht**, F. Sadikin, B. Stanley, E. Ayturk

BIOT 299. Experimental and theoretical studies of protein adsorption onto ion exchange and mixed mode chromatographic column packings. **D. Frey**, M.M. El-Sayed, P. Rezaei

BIOT 300. Evaluation of five commercial immunoassays for quantification of leaked ligand from a new protein A resin. **E. Monie**, T. Bjorkman, A. Forss

BIOT 301. Packing CHT™ resin in a one meter pack-in-place Pall Resolute® manual column: Understanding the impact of shear on fine generation and column pressure performance. **E. Baragar**

BIOT 302. Particle size and ligand density effects on anion exchange chromatography behaviour for therapeutic protein manufacture. **G. Jasulaityte**, P. Gilbert, H.J. Johansson, D.G. Bracewell

BIOT 303. Withdrawn

BIOT 304. Novel technology for continuous manufacturing of agarose-based, monodisperse, chromatography beads. **H.J. Johansson**, P. Gilbert

BIOT 305. Enrichment of the components responsible for PS20 degradation. **J. Gu**, Y. Yigzaw

BIOT 306. Insights into the effect of pH on mAb surface properties and selectivity in multimodal chromatography systems. **J. Robinson**, S.M. Cramer

BIOT 307. Evaluating wash strategies to remove residual cell culture flocculant interactions with protein A chromatography resin. **K. Sing**, M. Peck, A. Schadock-Hewitt, N. Singh, S. Chollangi

BIOT 308. MAb aggregate removal with CEX flow-through frontal chromatography. **K.A. Cotoni**, M. Stone

BIOT 309. Use of a continuous chromatography system for both resin screening and scale-up studies. **L. Mathiasson**, **L. Persson**, **M. Berg**, M. Hall, **H. Blom**, A. Ljunglöf, B. Westerlund, **H. Nordvarg**, **C. Fenge**

BIOT 310. Design space development for mAb ProA chromatography and VI. **L. Gonzalez**

BIOT 311. Improving production efficiency through overload chromatography. **M. Wong**, J. Brown, J. Yang, D. Glover, C. Williams, Y. Yigzaw

BIOT 312. Continuous chromatography solutions and the effect of number of columns on process performance. **M. Pagkaliwangan**, X. Gjoka, R. Gantier, M. Schofield

BIOT 313. New protein L affinity resins

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for antibody fragments purification. **M. Hanamura**, S. Nakamura, J. Yasuoka, K. Yoshimura

BIOT 314. Continuous multi-column chromatography: Methodology for the selection of the most suitable protein A media. **M. Higson**, M. Holstein, C. Gillespie

BIOT 315. Purification of cell culture-derived oncolytic measles virus by membrane chromatography. K. Lothert, D. Loewe, T. Grein, P. Czermak, **M.W. Wolff**

BIOT 316. High throughput resin selection for the recovery of valuable compounds from food products. **M. Moreno Gonzalez**, V. Grish, P. Chuekitkumchorn, G. Ferreira, H. Wijngaard, M. Ottens

BIOT 317. Increasing continuous purification productivity by combining small particle size chromatography resin with continuous countercurrent tangential chromatography (CCTC). **O. Shinkazh**

BIOT 318. Implementation of directly scalable single-use protein A chromatography for rapid processing from bench to industrial processing. **O. Hardick**, D.G. Bracewell, W. Lewis

BIOT 319. Withdrawn

BIOT 320. Formation of on-column aggregates during cation exchange chromatography and studies of its elimination. **R.B. Wollacott**, C. Connelly, S. Ozturk

BIOT 321. Use of activated carbon as an adsorbent in polishing step. **R. Skudas**

BIOT 322. Investigation into molecular basis of protein interactions in multimodal chromatography using nuclear magnetic resonance spectroscopy and molecular dynamics simulations. **R.B. Gudhka**, C. Bilodeau, S.A. McCallum, S.M. Cramer

BIOT 323. High-throughput screening for purification development of osteospontin-an acidic recombinant protein expressed in *E. coli*. **S. Guo**, A. Ravi, S. Mayfield, Z.L. Nikolov

BIOT 324. Investigation into the different mechanisms of interaction in multimodal anion and multimodal cation exchange systems. **S. Parasnavis**, J. Robinson, S.M. Cramer

BIOT 325. Fine-tuning your purification process: Using mechanistic modeling of chromatography to optimize the balance between yield, purity, and ease of operation. **T.J. Fattor**, S. Hunt, J. Rocher, R.J. Todd

BIOT 326. Comparative study of commercially available protein A chromatography resins and Amsphere™ A3: Qualitative analysis of residual host cell proteins by means of 2D-LC/MS. **T. Shiotani**, S. Tsuda, T. Tanaka, M. Hanamura, M. Nagaya

BIOT 327. Single-molecule and isocratic protein competition on ion-exchange adsorbents. **U. Patil**, L. Kisley, S.P. Dhamane, M. Poongavanam, A. Mansur, S. Dominguez Medina, E. Kulla, J. Chen, L.J. Tauzin, K. Kourentzi, C.F. Landes, R.C. Willson

BIOT 328. In situ analysis of ligand density on the surface of regenerated cellulose membranes. **V. Bansal**, E. Fasoli, J.O. Sotero Esteva, I.J. Dmochowski

BIOT 329. Optimisation of preparative polishing chromatography for a ternary antibody mixture. **V. Fischer**, R. Kucia-Tran, W. Lewis, A. Velayudhan

BIOT 330. Withdrawn

BIOT 331. Leveraging innovative technologies for cost-effective protein A chromatography operation. **Y. Brodsky**, E. Gefroh, M. McClure, R. Piper, L. Connell-Crowley

BIOT 332. Systemic approach to remove host cell proteins during monoclonal antibody protein A chromatography. **Z. Xia**, Y. Zhou, Y. Wu

BIOT 333. Linear scalablity of Planova BioEX and Planova 20N filters. **A. Shah**, B. Buesing, D. Strauss, N. Hirotomi, T. Miyabayashi

BIOT 334. Evaluation of virus filtration prefilters and load conditions for a highly fouling mAb. **H. Keefe**, N. Bennett, S. Sargis, A. Seay

BIOT 335. Synthesis of well-defined and easily functionalized copolymers for the preparation of lipid-disc cell membrane mimetics. **K. Burridge**, I. Sahu, A. Craig, E. Clark, S. Al-Abdul-Wahid, M. Dolan, C. Dabney-Smith, D. Konkolewicz, G. Lorigan

BIOT 336. Nanocellulose-based size exclusion filters as an efficient and convenient virus barrier filter. **L. Manukyan**, A. Mihranyan

BIOT 337. Exploration of synthetic depth filtration applied to mammalian cell harvest. **P. Kalashnikov**

BIOT 338. Comparison of DSC cryoporomtery and liquid-liquid porometry for validation of pore size distributions of nanocellulose-based virus removal filter papers. **S. Gustafsson**, A. Mihranyan, L. Roemer

BIOT 339. Investigation of particle size distribution for CHO cell culture media filtration. **T. Ito**, K. Chan, Y. Tomioka, A. Cheong, Y. Mok

BIOT 340. Considerations for bulk fill filtration of high concentration drug substance. **T. Parker**, C. Nieder

BIOT 341. Clarification of a pre-treated mAb-producing harvest using new fully synthetic depth filter technology. V. Medvedev, **Y. Cherradi**, S. Le Merdy, T. Albano

BIOT 342. Introduction and removal of β-glucans in a biological purification process: A case study. **A. Pearson**, R. Luo, K.E. Goklen

BIOT 343. Demonstrating robust clearance of beta-glucans in an E. coli purification process. **A. Morris**, A. Nguyen Dang, A. Ladiwala, T. Peram

BIOT 344. Optimization of a multi-level flow rate loading trajectory. **A. Sellberg**, N. Andersson, A. Löfgren, **B. Nilsson**

BIOT 345. Comparison of charge variant methodologies for evaluating protein compatibility with dextrose infusion solutions. **B. Demirdirek**, J. Valente, W. Lan, M. Bolgar

BIOT 346. Use of high-throughput screening technology to develop flow through aggregate removal platforms. **C. Kittinger**, B.D. Gastfriend, K. Newell, E. O'Connor, V. Riguero

BIOT 347. Centre-cut separation of biomolecules by stepwise-elution SMB. **C. Wayne**, A. Velayudhan

BIOT 348. Manipulating the selectivity of ceramic hydroxyapatite (CHT) for acidic protein purification. **L. Vang**, X. He

BIOT 349. Utilizing single use (SU) technology for single pass (SP) TFF operations. **E. Peterson**

BIOT 350. Design and integration of in situ liquid liquid extraction systems for bioacid production. P. Saboe, L. Manker, G. Beckham, **E. Karp**

BIOT 351. Di-block copolymer and enzyme conjugated nano layers: A packing density study to design bio-reactive membranes for water purification applications. **J. Pazol**, E. Nicolau

BIOT 352. Case study for evaluation of the 3M™ Emphaze™ AEX hybrid purifier involving low isoelectric point target proteins. **J. Pate**, B. Kester, C. Berdugo, Y. Li, V. Vinci

BIOT 353. Case study: Commercial-scale microbial control validation during centrifuge harvest operations. **K. Saldanha**

BIOT 354. Implementation of disposable technologies in support of closed processing and viral segregation for downstream clinical manufacturing. **K. Mattia**, B. Vu, P.R. Smith, A.R. Ubiera

BIOT 355. Reoxidation of reduced monoclonal antibody using modified downstream processing. **M. Moynihan**, J. Lutje, P.J. Alfonso, P. Singh

BIOT 356. Antisense oligonucleotide purification process: Successes and challenges during scale-up. **R. Gronke**, R. Joshi, H. Nguyen, Y. Fillon, K. Ruanjaikaen, F. Antia

BIOT 357. Downstream process development and transfer to cGMP manufacturing of novel fusion protein at CMC biologics. **S.C. Vilardi**

BIOT 358. Use safe light during biologics manufacturing, handling and storage. **C. Du**, A. Borwankar, A.T. Lewandowski, N. Singh, S. Ghose, M.C. Borys, Z. Li

BIOT 359. Performance of simultaneous single-pass concentration and diafiltration of protein solution using Pall Cadence™ inline diafiltration module. **B. Trafton**, **C. Matthews**

BIOT 360. Accelerating advancement in gene therapy by improving downstream purification of viral vectors. **O. Terova**

BIOT 361. Effect of mRNA structure on chromatographic performance. **M. Shamashkin**, M. Scott, H. Pujar

BIOT 362. Impact of multimodal cation-exchange chromatography on impurity separation of non-platform proteins. **E. Ayturk**, K. Selvitelli, M. Westoby

BIOT 363. Virus detection using restricted-access adsorbents. **U. Patil**, S.P. Dhamane, M. Adhikari, A. Hagstrom, U. Strych, K. Kourentzi, R.C. Willson

BIOT 364. Characterization of flow mechanics in a scaled down continuous viral inactivation reactor. **M. Brown**, L. Amarikwa, S. Parker, S.S. Yildirim, S. Godfrey, R. Orozco, J.L. Coffman

BIOT 365. Straight-through processing of insulin-like peptides. **P. Tiainen**, A. Löfgren, B. Nilsson

BIOT 366. Surface characterization and identification of optimum mixing conditions for protein solutions. A. Sokolnicki, **G. Raja**, S. Liao

BIOT 367. Analytical comparability strategies for biosimilars. **A. Schwendeman**

BIOT 368. Mechanistic understanding of the degassing phenomenon of drug products. **F. Schlegel**, C. Padala

BIOT 369. Adalimumab like biosimilar purification with ion exchange and mixed-mode resins. **R. Drevland**

BIOT 370. Effect of low pH transition wash on protein A eluate-mitigation strategy to improve manufacturing filterability. **J. Huerta**, W. Sun, I. Ramos

BIOT 371. Withdrawn

BIOT 372. Withdrawn

BIOT 373. Development of cost-efficient processes for adenovirus purification. **M. Bergman**, M. Bennemo, Å. Hagner-McWhirter, A. Akerblom, S. Häggblad-Sahlberg, E. Wallby, G. Ahlén, M. Lundgren

BIOT 374. High-throughput droplet tracking and automated image analysis in microfluidic device. **M. Vaithiyanathan**, K. R Bajgiran, P. Darapaneni, J.A. Dorman, A.T. Melvin

BIOT 375. Withdrawn

BIOT 376. Development of mathematical models to identify the fouling mechanism in depth filters for cell culture clarification. D. Jang, M. Peck, N. Singh, **A. Arunkumar**, S. Ghose, Z. Li

BIOT 377. Process simulations in a clinical scale single-use TFF system examine blend time efficiency. **A. Sokolnicki**

BIOT 378. Scalability model for mixing cell culture media in single-use GMP bioprocessing equipment. **A. Hansen**

BIOT 379. Increasing efficiency in bioprocessing using available software functions in a process automation approach. M. Pitkanen, **A. Morrison**, **T. Bjorkman**, **A. Graanberg**, **K. Lenberg**, **F. Lundström**

BIOT 380. Machine learning approaches for streamlining downstream process development. **D. Lee**, B. Tran

BIOT 381. Role of simulation and scheduling tools in bioprocess development and manufacturing. **D. Petrides**, D. Carmichael, C.A. Siletti

BIOT 382. Biomaterial production

‡*Cooperative Cosponsorship*

process intensification and analysis and optimization with process simulation tools. **D. Petrides**, D. Carmichael, C.A. Siletti

BIOT 383. Advanced process optimization–a novel, in-situ real time adaptive control system to accelerate and optimize biologics process development and manufacturing. G. Emmerson, S. Watts, S. Saxby, **G.E. Barringer**

BIOT 384. Process economics of continuous bioprocessing. **J. Hummel**, M. Pagkaliwangan, X. Gjoka, T. Davidovits, R. Stock, T. Ransohoff, R. Gantier, M. Schofield

BIOT 385. Copper catalyzed fragmentation of an IgG1 recombinant monoclonal antibody for therapeutic use: using kinetic modeling to fit process to product during technology transfer. **M. Henry**, G. Alkire, J.R. Molek, A. Szkodny, M. Monck, D.P. Nesta

BIOT 386. Use of modelization and scale-down models to support drug product development and transfer to manufacturing facilities: Challenges and benefits. **M. Belkacem**, C. De Kesel

BIOT 387. Enhancing multivariate calibration model reproducibility used for the online monitoring of upstream processes in continuous biomanufacturing. **N. Trunfio**, B. Chavez, S. Velugula, S. Yoon, C. Agarabi

BIOT 388. Development of QbD expertise among scientists in a biopharm product and process development organization. **S. Parimal**, P.R. Smith, S. Weisser, G.J. Terfloth, K.E. Goklen

BIOT 389. Near-infrared (NIR) spectroscopic analysis of water in lyophilized products for process efficiency improvements. **A. Hopkins**

BIOT 390. Best practices when developing a point of use pressure decay test. **A. Steele**

BIOT 391. At-line mass spectrometry-based process analytical technology for linking nutrient consumption and bioreactor product quality. **D.N. Powers**, N. Trunfio, E. Berilla, B. Chavez, C. Kohnhorst, S. Velugula, C. Agarabi

BIOT 392. EDTA determination in bovine serum albumin. **N. Gupta**, C. Felice, B. Ramanathan, K. Pipkins, J. Cunningham

BIOT 393. In-line cell culture analytics for high-throughput process development: An evaluation of the integrated FLEX2 bioanalyzer. **P. Liu**, M. Manahan, L. Hoshan, J. Pollard

BIOT 394. Detection and characterization of mycoplasma contamination in cell culture with application of nucleic acid testing assays. **T. Faison**, C. Kohnhorst, S. Velugula, E. Berilla, S. Lute, C. Agarabi, K.A. Brorson, J. Wang, S. Johnson

BIOT 395. Purification of PLBL2 critical reagent for ELISA development. **L. Wong**, P. McKay, J. Franklin

BIOT 396. *In silico* design and *in vivo* selection of riboswitches for cell-based detection of explosive compounds. **S. Harbaugh**, Y. Chushak, J. Martin, H. Salis, M. Goodson, J.L. Chavez, N. Kelley-Loughnane

BIOT 397. At-line investigation of capacitance for assessing biomass of mammalian cell culture. **K. Ramer**, J. Fernandes, A. Zhang, J. Currie

BIOT 398. Protein and cell–surface interactions and layer properties using MP-SPR. **A. Jarvinen**, N. Granqvist, J. Kuncova-Kallio

BIOT 399. Deoxyribozyme cascade for visual detection of Zika virus RNA. **A.J. Reed**, R. Connelly, A. Williams, H. Choe, Y. Gerasimova

BIOT 400. Using engineered zinc finger proteins to detect pathogen-specific DNA. **C. Sedlak**, M. Kim

BIOT 401. Forensic study: Differentiating and analyzing variances using microbiota to investigate home invasions. **C. Young**, D. Martin, C. Porter, V. Goss, J. Hampton–Marcell

BIOT 402. Visual split peroxidase-like deoxyribozyme probes for the detection of rifampin-resistance in *Mycobacterium tuberculosis*. **C. Verduzco**, Y. Gerasimova, R. Connelly

BIOT 403. Advances in the characterization of protein catalyzed capture (PCC) agents for robust biosensing. **C. Jones**, M. Coppock

BIOT 404. The fluorescence quenching ability of graphene oxide as a platform for pathogenic double-stranded DNA sensing utilizing engineered zinc finger protein. **D. Ha**

BIOT 405. Direct detection of double-stranded DNA of a pathogenic strain of STEC (Shiga toxin-producing *Escherichia coli*) using engineered zinc finger protein immobilized on paramagnetic beads. **J. Shim**, B. Kim, M. Kim

BIOT 406. Strategies for controlled bacterial assembly resulting in activation of a quorum-sensing circuit. **M.T. Kozlowski**, B.R. Silverman, C.P. Johnstone, D.A. Tirrell

BIOT 407. Real time detection of NASBA product by Split DNA aptameric sensor. **N. Kikuchi**, D.M. Kolpashchikov

BIOT 408. Design and fabrication of a triple-input microfluidic droplet trapping array towards multiplexed cancer diagnostics. **R. Elkhanoufi**, K. R Bajgiran, M. Vaithiyanathan, J.A. Dorman, A.T. Melvin

BIOT 409. Identifying peptide affinity ligands to demonstrate selectivity between dermal fibroblasts and endothelial cells. **R. Ghosh**, A. Mullerpatan, T. Baltazar, C. Catarino, A. Nascimento, P. Karande, S.M. Cramer

BIOT 410. Split deoxyribozyme probe for efficient interrogation of highly structured RNA targets. **S. Solarez**, Y. Gerasimova

BIOT 411. Developing a genetically-encoded insulin sensor for live imaging: Application to Alzheimer's disease. **S.S. Raza**, W. Chen

BIOT 412. SBAP-linked bioconjugation of oligonucleotides to quantum dots. B. Eichler, **T. Hollinsworth**, **A. Kroeger**

BIOT 413. Mutation detection of RNA in extracellular vesicles with a cationic lipoplex nanoparticle biochip. **Y. Sheng**, J. Hu, L.J. Lee

BIOT 414. Highly sensitive programmable RNA detection using fluorescent RNA aptamer. **Y. Furuhata**, M. Kobayahshi, R. Maruyama, Y. Sato, K. Makino, T. Michiue, H. Yui, S. Nishizawa, K. Yoshimoto

BIOT 415. Characterization of nitric oxide flux as a function of time and temperature: A durability review. **M.M. Jeakle**

BIOT 416. Kinetic characterization and differentiation of atrazine catabolism via *Pseudomonas* sp. strain ADP biofilms and planktonic cells. **M. Delcau**, T.L. Peeples

BIOT 417. Microfluidic device to characterize the effect of orthogonal chemical gradients on 3D cancer cell migration. **J.M. Campbell**, S. Rahman, A.T. Melvin

BIOT 418. Withdrawn

BIOT 419. Microfluidic co-culture of breast cancer cells and adipose stem cells. **S. Rahman**, K. Render, J.M. Campbell, E. Martin, A.T. Melvin

BIOT 420. Examine how oscillating patterns of chemical gradients break the spatial range limitations of conventional chemotaxis. **S. Rahman**, J.M. Campbell, I. Schneider, A.T. Melvin

BIOT 421. Developing a high affinity, dynamic scaffold toolkit for control of intracellular metabolic flux. **A.A. Mitkas**, W. Chen

BIOT 422. Alcoholic liver damage prevention of *Moringa oleifera* extract. **J. Park**, C. Kim, S. Oh, S. Chang, K. Shin

BIOT 423. Probing protein-ice interactions using high resolution synchrotron X-ray diffraction. **B. Bhatnagar**, **X. Wen**, B. Zakharov, A. Fisyuk, F. Karim, K.J. Quach, I. Seretkin, A. Fitch, E. Boldyreva, E. Shalaev

BIOT 424. Isolation and characterization of the EphA2 cytoplasmic domains. **J. Shirkey**, P. Gil-Rodriguez, M. Buck

BIOT 425. Confocal Raman microscopy investigation of cytochrome c-phospholipid interactions which induce permeability in mixed phospholipid vesicle membranes. **J.P. Kitt**, D. Bryce, S.D. Minteer, J.M. Harris

BIOT 426. Contribution of the C-terminus to $A_{2A}R$ activity and stability. **K. Swonger**, A.S. Robinson

BIOT 427. Excipient choice for protection against metal-catalyzed oxidation: Impact of chelator on stability of biologic drug products. **M.E. Krause**, T. Haby, S. Patke, M. Bolgar, M. Huang, L. Breckenridge, M. Khossravi

BIOT 428. Synthesis of new β-amino acids derivatives as anti *trypanocidal* agent and docking & Inhibition study on *trans-sialidase* enzyme. **M. Kashif**, M. Ashfaq, G. Reveria

BIOT 429. Folding analysis of bovine pancreatic trypsin inhibitor (BPTI) with aromatic thiols and disulfides *in vitro*. **N. Zhang**, R. Marahatta, W.J. Lees

BIOT 430. Prediction and characterization of the equilibrium ensembles of TGF-β3 using bias exchange metadynamics. **R. Singh**, G. Goel

BIOT 431. In silico study of dimer association of insulin during aggregation. **R.P. Mishra**, R. Singh, T. Rao, G. Goel

BIOT 432. Divalent metal ion-independent cell adhesion events mediated by E-cadherin-binding DNA aptamer that forms parallel type G-quadruplex with three long loops. **R. Maruyama**, T. Yoshitomi, F. Wayama, K. Wakui, K. Makabe, H. Furusho, K. Yoshimoto

BIOT 433. Extraction of protein thermodynamic parameters from high-throughput differential scanning fluorimetry assays. **T.A. Wright**, J. Stewart, D. Konkolewicz, R.C. Page

BIOT 434. DNA cleavage via prokaryote argonaute mediated by an uncharacterized N-terminal domain. **K.Z. Lee**, A. Liu, A. Kikla, K. Solomon

BIOT 435. Insights from molecular dynamics simulations into the structure and dynamics of ITPA mutants. **Y.A. Houndonougbo**

BIOT 436. Understanding co-solutes effects on viscosity and protein interactions in highly concentrated monoclonal antibodies through protein structure and dynamics. **J. Hung**, B. Dear, W. Zeno, C. Karouta, M. Nieto, L. Wilks, A. Sharma, J. Stachowiak, T. Truskett, K.P. Johnston

BIOT 437. Facile preparation of covalent C-to-C linked nanobody fusions by freezing. **B. Zang**, L. Jia, J. Ren, Q. Peng

BIOT 438. Fluoroalcohol-induced coacervation in membrane proteomics. **R.R. Rion**, A. Oloumi, M. Azizi, A. Koolivand, M. Khaledi

BIOT 439. Remodeling of a human microbiome model. **A.M. Bhagwat**, C.H. Collins, J.S. Dordick

BIOT 440. Phosphoproteomic and transcriptomic analysis of cell wall stress response in *Aspergillus nidulans* reveals novel cell wall integrity signaling proteins. **C. Chelius**, K. Boppidi, S. Lincoln, J. Kumar, S. Reese, S. Hossain, D. Thomas, K. Lawson, J. Ramsey, A. Ramsey, R. Srivastava, S. Harris, M. Marten

BIOT 441. Effects of buffer condition on the hydrodynamic radius of biomolecules. **F. Rong**, N. Khereid, S. Wickramasinghe, **X. Qian**

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

WEDNESDAY MORNING

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Advances in Non-Chromatographic Separations: Depth Filtration and UF/DF Operations

L.W. Pampel, N. Sanaie, *Organizers*

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D.W. Wood, *Organizer, Presiding*
R. Sheth, A.L. Zydney, *Presiding*

8:30 BIOT 442. Downstream process impact of reducing impurities during harvest operations using charged hybrid filters. **B. Kluck**, C. Tran, A. Voloshin, E. Ozcam, B. Dransart, R. Krishnan

8:50 BIOT 443. Evaluation of the effects on HCP clearance and other impurities of mPAA and all-synthetic depth filters (X0SP). **H.C. Nguyen**, Y. Tao, W.R. Emery, M.K. Paik

9:10 BIOT 444. Mechanisms of DNA retention on depth filters. **O. Khanal**, N. Singh, S.J. Traylor, X. Xu, S. Ghose, A.M. Lenhoff

9:30 BIOT 445. Mechanistic modeling of the loss of protein sieving due to internal and external fouling of microfilters. **A. Apostolidis**, G. Bolton

9:50 Intermission.

10:10 BIOT 446. Effect of zinc chloride and PEG concentrations on the critical flux during tangential and normal flow microfiltration of BSA precipitates. **Z. Li**, A.L. Zydney

10:30 BIOT 447. UF/DF processes for high concentration mAb formulations: Reconciling process development and evolving trends. **A. Arunkumar**, N. Singh, S. Ghose, Z. Li

10:50 BIOT 448. Evaluation of single-use TFF technologies for high concentration operations. **V. Adams**, T. Parker

11:10 BIOT 449. Understanding the sterile filtration of nanosuspensions. **K. Zourna**, J.H. Welsh

Section A
InterContinental New Orleans
La Salle A

BIOT Awards

Biotechnology & Bioengineering Elmer Gaden Award Lecture

M.R. Antoniewicz, N. Tugcu, *Organizers*
T.M. Przybycien, *Organizer, Presiding*

11:30 Introductory Remarks.

11:35 BIOT 450. Barrier tissue mimics for drug development. **M.L. Shuler**

Section B
InterContinental New Orleans
La Salle B/C

End-to-End Biomanufacturing

Disruptive Bioprocessing & Process Integration

S.W. Harcum, V. Natarajan, N. Rathore, S.A. Tobler, *Organizers*
A. Hewig, A.M. Lenhoff, M. Westoby, *Presiding*

8:30 BIOT 451. Withdrawn

8:50 BIOT 452. Upstream optimization and non-chromatographic downstream strategy for production and purification of antimicrobial peptide in *E. coli*. **M. Joachim**, T. Weidner, D. Gerlach, P. Czermak

9:10 BIOT 453. Innovating biopharmaceutical manufacturing for an age of acceleration. **J.C. Love**

9:50 Intermission.

10:10 BIOT 454. Developing an end to end bio-manufacturing platform for the new paradigm of SAM (Self Amplifying mRNA vaccines). **V. Roy**, M. Bugno, D. Chinchilla-Olszar, K. Forney-Stevens, M. Xie, L. Harrington, C. Baldwin, N. Delahaye, J. Ulmer, K. Aggarwal, D. O'Hagan

10:30 BIOT 455. Techno-economic analysis of semicontinuous production of recombinant butyrylcholinesterase in transgenic rice cell suspension cultures. **J. Corbin**, K. McDonald, S. Nandi

10:50 BIOT 456. Use of a carbon footprint calculation to assess the environment impact of drug substance manufacture in GSK biopharm. **P.R. Smith**, M. Snyder, K. Kahle, K. Tomko, A. Adams, M. Schaad, D. D'Aquila

11:10 BIOT 457. Next-generation vaccine facility: Merging high productivity technologies for robust and cost-effective manufacturing. **R. Jacquemart**, J. Castillo, C. Yallop

Section C
InterContinental New Orleans
Pelican I/II

Biomedical & Emerging Technologies

New Strategies for the Delivery of Therapeutics: From Proteins & Genes to Cells

A.M. Kloxin, A. Noyes, J.P. Pieracci, *Organizers*
P. Mallikaratchy, J. Pieracci, *Presiding*

8:30 BIOT 458. Controlled EGFR ligand display on cancer suicide enzymes for targeted intracellular delivery. **R. Lieser**, M.O. Sullivan, W. Chen

8:50 BIOT 459. Enhanced cellular delivery of enzymes using the cowpea chlorotic mottle virus. **M. de Ruiter**, J.J. Cornelissen

9:10 BIOT 460. Novel microfluidic system for encapsulation of equine endothelial colony forming cells for local cell delivery. **Y. Tian**, W.J. Seeto, R. Winter, F. Caldwell, A. Wooldridge, E.A. Lipke

9:30 BIOT 461. Peptoid-based coatings as artificial extracellular matrix for increased differentiation of human embryonic stem cells into neural cells. **J. Roberts**, G. Perez, M. Borrelli, S.L. Servoss

9:50 Intermission.

10:10 BIOT 462. D-VITylation: Harnessing the biology of vitamin D to improve the pharmacokinetic properties of peptides and small proteins. **D.B. Hall**, A.S. Vakkasoglu, C.W. Hill, L.M. Hales, T.M. Soliman

10:30 BIOT 463. Bioengineered injectable thermogel for intravitreal protein controlled release to the retina. **V. Delplace**, E. Tsai, A. Ortin-Martinez, M. Pakulska, V. Wallace, M.S. Shoichet

10:50 BIOT 464. Wavelength-specific, plasmonic nanoparticle mediated rupture of polymersomes using ultrafast single-pulse irradiation. **J.C. Griepenburg**, A.R. Robinson, G.M. Disalvo, S.M. O'Malley, D.M. Bubb

11:10 BIOT 465. Cheminformatics-driven discovery of polymeric micelle formulations of poorly soluble drugs. **E. Muratov**, V.M. Alves, D. Hwang, M. Sokolsky, E. Lebed, N. Vinod, C. Andrade, A. Kabanov, A. Tropsha

Section D
InterContinental New Orleans
Frenchman Ballroom

Upstream Processes

Synthetic Biology

Cosponsored by WCC
R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
T.J. Mansell, Y. Yoshikuni, *Presiding*

8:30 BIOT 466. MinGenome: Top-down synthesis of genome minimized strains for bioproduction. **L. Wang**, C. Maranas

8:50 BIOT 467. MODCELL: A prototype for modular cell engineering. **C.T. Trinh**

9:10 BIOT 468. Single-pot glycoprotein biosynthesis using a cell-free transcription-translation system enriched with glycosylation machinery. **T. Jaroentomeechai**, J.C. Stark, M.C. Jewett, M.P. DeLisa

9:30 BIOT 469. Engineering synthetic consortia inspired by the rumen microbiome. **M.A. O'Malley**

9:50 Intermission.

10:10 BIOT 470. Operon refactoring and construction assistant (ORCA): An integrated workflow to refactoring biosynthetic gene clusters. **E. Oberortner**, M. Wornow, M. Hadjithomas, S. Deutsch

10:30 BIOT 471. Engineering species-like barriers to sexual reproduction for applications in public health, agriculture, and the environment. **M. Smanski**

10:50 BIOT 472. Optimization, evolution, and control of pathways and metabolism in yeasts. **H.S. Alper**

WEDNESDAY AFTERNOON

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Advances in Non-Chromatographic Separations: Precipitation & Viral Filtration

L.W. Pampel, N. Sanaie, *Organizers*
D.W. Wood, *Organizer, Presiding*
R. Sheth, A.L. Zydney, *Presiding*

2:00 BIOT 473. Development of a method for purification of monoclonal antibodies utilizing precipitation. **A. Mutchler**

2:20 BIOT 474. Water on hydrophobic surfaces – modeling of precipitation. **S. Grosshans**, G. Wang, J. Hubbuch

2:40 BIOT 475. Single-step purification of small non-mAb biologics by peptide-ELP based affinity precipitation. **A. Mullerpatan**, A. Nascimento, R. Ghosh, E. Kane, P. Karande, S.M. Cramer

3:00 BIOT 476. One-step affinity capture and precipitation for enhanced purification of mAbs and Fc-fusion proteins using Z-ELP functionalized nanocages. **A. Swartz**, X. Xu, S.J. Traylor, Z. Li, W. Chen

3:20 Intermission.

3:40 BIOT 477. Optimization of downstream purification for Modified Vaccinia Ankara virus. L. Thomas, **A. Xenopoulos**, U. Reichl, M.W. Wolff

4:00 BIOT 478. Understanding virus removal filtration in nanocellulose-based filter paper. **A. Mihranyan**

4:20 BIOT 479. Challenges of implementing virus filtration into continuous manufacturing processes. **D. Strauss**, K. Kobayashi, N. Hirotomi

4:40 BIOT 480. The effects of buffer condition on viral clearance of model proteins. N. Khereid, F. Rong, D. Sasongko, S. Wickramasinghe, **X. Qian**

Section B
InterContinental New Orleans
La Salle B/C

Upstream Processes

Mammalian Cell Culture & Engineering: Perfusion Cultures for Scale up and Production

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
Y. Cho, N. Jacob, S. Ozturk, A.B. Tolstrup, *Presiding*

2:00 BIOT 481. Continuous processing: Lessons learned from the past and strategies for success in the future. **S. Ozturk**

2:20 BIOT 482. Development of a statistical model to support perfusion bioreactor scale-up. **K. Schwarz**, J. Raley

2:40 BIOT 483. Understanding product sieving challenges in TFF perfusion cell culture and developing strategies for mitigation. **L. Sawicki**, D. Ogawa, H. Tessman, F. Strefling, S. Godfrey, J.L. Coffman, T. Luman, H. Lin, M. Yu

3:00 BIOT 484. Computational fluid dynamic modeling and design of a novel single-use airlift perfusion reactor prototype for human cells. **C. Doris**, C. Bardliving, P. Shamlou

3:20 Intermission.

3:40 BIOT 485. Optimizing the addition antifoam for process intensification: A case study using small scale models. **J. Wang**, J. Walther

4:00 BIOT 486. Process improvement of a high density fed-batch process using N-1 perfusion seed cultures. **J. Yee**, T. Erlandson, S. Ray, S. Sowa, J. Tian, Q. He, M.C. Borys, Z. Li

4:20 BIOT 487. A novel high density N-1 batch seed strategy development for CHO cell culture manufacturing. **A. Yongky**, J. Zhao, J. Xu, M. Rehmann, M.C. Borys, Z. Li

4:40 BIOT 488. Development and implementation of perfusion N-1 for mammalian cell culture to enhance process productivity. **R. Sanford**

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Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Prediction & Characterization of Biophysical Properties of Proteins

E. Sahin, P.M. Tessier, *Organizers*
M. Ottens, J. Perchiacca, A. Schwendeman, *Presiding*

2:00 BIOT 489. Prediction of protein biophysical properties and chemical modifications by correlating in silico protein structural features. **L. Jia**, D. Toledo Warshaviak, Y. Sun

2:20 BIOT 490. Insulin folding landscape and in-silico design of peptide excipients to inhibit aggregation. **G. Goel**, R. Singh, A. Mishra, R. Bansal, A.S. Rathore

2:40 BIOT 491. Predicting pH and ionic strength effects on the colloidal stability of antibodies. **M.A. Blanco**, H.W. Hatch, M. Castellanos, C.W. Meuse, K.W. Mattison, I. Karageorgos, J.E. Curtis, V.K. Shen

3:00 BIOT 492. Experimental and bioinformatics methods for identifying monovalent and bivalent antibodies with high colloidal stability. **M.E. Alam**, S.B. Geng, C. Bender, S.D. Ludwig, L. Linden, R. Hoet, P. Tessier

3:20 Intermission.

3:40 BIOT 493. Predicting the solubility of VLPs: Qualitative structure property relationship (QSPR) modeling applied to HBcAg VLPs. **P. Vormittag**, C. Dürr, A. Wilming, T. Hiller, T. Klamp, J. Hubbuch

4:00 BIOT 494. Characterizing long-term protein phase behavior via multidimensional empirical protein phase diagrams containing image-based features. **M. Klijn**, J. Hubbuch

4:20 BIOT 495. Protein-protein interactions and viscosity of highly concentrated monoclonal antibody solutions. **B. Dear**, J. Hung, J. Bollinger, L. Wilks, A. Sharma, C. Karouta, M. Nieto, T. Truskett, K.P. Johnston

4:40 BIOT 496. Microrheology of antibody solutions. **E.M. Furst**, M. Woldeyes, C.J. Roberts

Section D
InterContinental New Orleans
Frenchman Ballroom

Biomedical & Emerging Technologies

New Strategies for the Delivery of Therapeutics: From Proteins & Genes to Cells

A.M. Kloxin, A. Noyes, J.P. Pieracci, *Organizers*
P. Mallikaratchy, J. Pieracci, *Presiding*

2:00 BIOT 497. Revoke immunosuppression of tumor microenvironment using engineered molecular traps. **R. Liu**, L. Miao, J. Li, L. Huang

2:20 BIOT 498. Driving targeted, reversible cell-cell interactions with a universal membrane engineering method. **C.M. Csizmar**, J.R. Petersburg, L.A. Stern, B.J. Hackel, C.R. Wagner

2:40 BIOT 499. Development of late-stage ready CMC approaches to enable recombinant AAV biomanufacturing. **K. Clark**

3:20 Intermission.

3:40 BIOT 500. Development of a scalable production process for the manufacturing of exosome-based biotherapeutics. **A. Noyes**, K. Ellis, M. Doherty, R. Bourdeau, M. Mercaldi, K. Konstantinov

4:00 BIOT 501. Hepatitis B viral-like particles as protein delivery vehicles for targeted therapy and genome editing. **E. Hartzell**, H. Kim, W. Chen

4:20 BIOT 502. Effective cancer therapy via therapeutic-loaded, cell-derived nanovesicles induced by sulfhydryl-blocking (NIbS). **D. Ingato**, J. Edson, M. Zakharian, Y.J. Kwon

4:40 BIOT 503. Incorporation of a weak poly(acid) into multilayer polymer coatings enables rapid contact-transfer of DNA to soft surfaces. **V. Appadoo**, Y. Yu, J. Ren, B. Liu, T. Hacker, D.M. Lynn

WEDNESDAY EVENING

Section A
InterContinental New Orleans
La Salle A

BIOT Awards

Biotechnology & Bioengineering Daniel I.C. Wang Award Lecture

M.R. Antoniewicz, N. Tugcu, *Organizers*
T.M. Przybycien, *Organizer, Presiding*

5:00 Introductory Remarks.

5:05 BIOT 504. Adventures in RNA synthetic biology. **C. Beisel**

THURSDAY MORNING

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Challenges in Downstream Technology Transfer & Novel Processing Implementation

L.W. Pampel, N. Sanaie, D.W. Wood, *Organizers*
M. Brower, B. Roman, *Presiding*

8:30 BIOT 505. Efficient technology transfers to increase agility, flexibility, and productivity. **A. Goerke**, K.A. Calhoun

8:50 BIOT 506. Effects of bed compression on protein separation on gel filtration chromatography at bench and pilot scale. **D. Kong**, S. Gerontas, R. McCluckie, M. Mewies, D. Gruber, N. Titchener-Hooker

9:10 BIOT 507. Development of in-line PAT tool for real-time concentration measurement of biologics during ultrafiltration/diafiltration. **S. Krishnan**, S. Sripada, S. Bose, D. Bhanushali

9:30 BIOT 508. A case study of tech transfer and growing pains: Shoehorning a process to fit a facility. **A. Henry**, L. Zhang, Y. Lam, J. Walker, D. McCann, M. Westoby, E.K. Koepf

9:50 Intermission.

10:10 BIOT 509. Scale up design and optimization for an intensified downstream process utilizing multi-column operations. **J.M. Angelo**, S. Chollangi, J. Pagano, D. Baur, K. Mihlbachler, T. Mueller-Spaeth, X. Xu, M. Morbidelli, S. Ghose

10:30 BIOT 510. Multi-column continuous chromatography as a strategy for reducing cost of drug development. **M. Najera**

10:50 BIOT 511. Technical and practical solutions to the challenges of low pressures and process interruptions in optimal continuous virus filtration. **N. Jackson**, K. Jones

11:10 BIOT 512. Investigation of biomimetic resin structure using CFD modeling of nano/meso fluid behavior for chromatographic gene therapy vector purification. **K. Vehar**, C. Bardliving, P. Shamlou

Section B
InterContinental New Orleans
La Salle B/C

End-to-End Biomanufacturing

Modeling Applications for Improved Process & Product Design

S.W. Harcum, V. Natarajan, N. Rathore, S.A. Tobler, *Organizers*
T.M. Przybycien, D.J. Roush, *Presiding*

8:30 BIOT 513. Towards automated model-based process development. **T. Hahn**, A. Papadopoulos, A. Gutzler, T. Huuk, T.C. Beck, J. Hubbuch

8:50 BIOT 514. Optimization of biologics process development enabled via data mining and quantitative structure analysis. **F.K. Insaidoo**, G. Stella, H. Li, N. Tugcu, D.J. Roush

9:10 BIOT 515. Modeling light transmission and chemistry in production-scale ultraviolet thin-film reactors. **R. Hart**

9:30 BIOT 516. Dependence of elution peak shape on binding models and resin structure in ion-exchange chromatography of proteins. **V. Kumar**, K. Westerberg, C. Kunert, F. Schlegel, A.M. Lenhoff

9:50 Intermission.

10:10 BIOT 517. Effects of protein and ligand structure on protein-multimodal ligand interactions in antibody systems. **C. Bilodeau**, E.Y. Lau, D.J. Roush, S. Garde, S.M. Cramer

10:30 BIOT 518. Development of a mechanistic model for the peristaltic pump filling unit operation to enable drug product process design. **J. Bernacki**, D. Marsiglio, N. Rathore, H. Rose

10:50 BIOT 519. Online monitoring of quantity, purity and potency of an antibody capture process. **N. Walch**, D. Sauer, E. Felföldi, T. Scharl-Hirsch, M. Melcher, F. Leisch, A. Jungbauer, A. Dürauer

11:10 BIOT 520. Application of biophysical and modeling tools for formulation and process development of biologics. **V. Antochshuk**

Section C
InterContinental New Orleans
Pelican I/II

Biomolecular & Biophysical Processes

Prediction & Characterization of Biophysical Properties of Proteins

E. Sahin, P.M. Tessier, *Organizers*
M. Ottens, J. Perchiacca, A. Schwendeman, *Presiding*

8:30 BIOT 521. Influence of different freeze and thaw ramps on the phase behavior of lysozyme from chicken egg white. **A.K. Wöll**, M. Desombre, L. Enghauser, J. Hubbuch

8:50 BIOT 522. Connecting protein conformation and dynamics with ligand-receptor binding using 3-color Förster resonance energy transfer tracking. **D. Marruecos**, M. Kastantin, N. Grover, S.Y. McLoughlin, D.K. Schwartz, J. Kaar

9:10 BIOT 523. Effect of polysorbate 20 and 80 on higher-order structure of a monoclonal antibody and its Fab and Fc fragments probed using 2D-NMR. S. Singh, **S. Bandi**, D. Jones, K. Mallela

9:30 BIOT 524. Establishing a pathway for robust implementation of higher order structure assessment of monoclonal antibodies therapeutics by 2D-NMR. **R.G. Brinson**, L.W. Arbogast, F. Delaglio, J.P. Marino

9:50 Intermission.

10:10 BIOT 525. Preferential interaction of osmolytes with IgG1 monoclonal antibodies. **C. Sudrik**, T. Cloutier, H.A. Sathish, B.L. Trout

10:30 BIOT 526. Single particle virus isoelectric point determination with chemical force microscopy. X. Mi, **C. Heldt**

10:50 BIOT 527. Bioengineered hydrogel models of Alzheimer's disease: Studying β-amyloid protein aggregation within 3D scaffolds. **L.W. Simpson**, J.B. Leach

11:10 BIOT 528. Integrating experimental and computational approaches to elucidate mechanisms of binding in multivalent proteins. W.J. Errington, B. Bruncsics, **C.A. Sarkar**

Section D
InterContinental New Orleans
Frenchman Ballroom

Upstream Processes

Engineering Natural Products Biosynthesis

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
K. Hawkins, M. Smanski, *Presiding*

8:30 BIOT 529. Expression of snake-antivenom peptide in *Pichia pastoris*. I. Juarez Contreras, S. Tang, C. Laperyi, K. Le, **C.F. Komives**

8:50 BIOT 530. Expression and *in vitro* reconstitution of novel lasso peptide gene clusters. **J.D. Koos**, A. Link

9:10 BIOT 531. New fungal RiPP family changes the rules for modified peptide

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biosynthesis. **M.F. Freeman**

9:30 BIOT 532. Enabling natural products discovery from anaerobic fungi via integrated 'omics' approaches. **C. Swift**, K. Louie, B. Bowen, K. Bingol, H. Heyman, T. Northen, M.A. O'Malley

9:50 Intermission.

10:10 BIOT 533. Redefining polyketide synthase modules. **A. Keatinge-Clay**, D. Vander Wood

10:30 BIOT 534. Nature as the ultimate combinatorial biosynthetic chemist: Inspiration for engineering natural products biosynthesis. **B. Shen**

10:50 BIOT 535. A synthetic biology approach to precursor-directed biosynthesis of complex polyketides and terpenes. **G.J. Williams**

11:10 BIOT 536. Engineering biosynthesis of the anticancer alkaloid noscapine in yeast. **Y. Li**

THURSDAY AFTERNOON

Section A
InterContinental New Orleans
La Salle A

Downstream Processing

Antibodies, Drug Conjugates & Novel Formats

L.W. Pampel, D.W. Wood, *Organizers*
N. Sanaie, *Organizer, Presiding*
E.T. Boder, A.M. Lenhoff, *Presiding*

2:00 BIOT 537. Assembly and purification of a novel format Fab'2 bispecific. **G. Giese**, A. Williams, J. Dvornicky, B. Tran, M. Fedesco

2:20 BIOT 538. Affinity capture options for monovalent bispecific antibodies. **M.T. Aspelund**, D. Gadre, T. Pabst, A.K. Hunter

2:40 BIOT 539. Integrated purification process development for the single-domain variable fragment of camelid antibodies. **C. Goodwine**, N. Vecchiarello, K. Love, J.C. Love, S.M. Cramer

3:00 BIOT 540. Resolution and enrichment of antibody fragments through pH modulation on an affinity chromatography step. **J. Woo**, N. Sanaie, R. Krishnan

3:20 Intermission.

3:40 BIOT 541. Strategies for achieving clearance of challenging host cell impurities in development of purification processes for biotherapeutics. **J.H. Lee**, A. Ladiwala, W. O'Dwyer, K. Shomglin, M. Butler

4:00 BIOT 542. Downstream process optimization to prevent fragmentation caused by cathepsin L. **N.E. Levy**, L. Madhavan, J.R. Molek, K.E. Goklen

4:20 BIOT 543. Engineering TNB (5-Thio-2-NitroBenzoic acid) on antibody to enable selective reduction. **A. Prashad**

4:40 BIOT 544. Effective removal of *Bacillus cereus* exotoxin by a two-step mAb chromatography process. **A. Graanberg**, S. Grönlund, T. Bjorkman, M. Wetterhall, S. Musunuri, K. Chaloupka, P. Gammell

Section B
InterContinental New Orleans
La Salle B/C

Upstream Processes

Engineering of Non-Model Systems

R.R. Kshirsagar, B. Pfleger, A. Russo, *Organizers*
A. Guss, J. McBride, C. Peebles, Z. Shao, *Presiding*

2:00 BIOT 545. Microdroplet-assisted evolution of *Yarrowia lipolytica* for the production of secreted riboflavin (vitamin B2). **J.M. Wagner**, L. Liu, S. Yuan, E. Williams, M. Venkataraman, A.R. Abate, H.S. Alper

2:20 BIOT 546. Discovery of metabolic pathways for lipid-production from lignin-derived phenolics in a non-model oleaginous yeast. **A. Yaguchi**, M. Spagnuolo, A. Robinson, E. Mihealsick, M.A. Blenner

2:40 BIOT 547. Global regulation of lignocellulolytic proteins from anaerobic fungi in response to substrate lignin content and composition. C. Hooker, M. Schacht, A. Hunnicutt, J. Overton, **K. Solomon**

3:00 BIOT 548. Elucidating core design principles to engineer nonconventional yeasts as novel microbial factories. **Z. Shao**, M. Cao, M. Gao, L. Zhao, W. Sun

3:20 Intermission.

3:40 BIOT 549. Developing the thermotolerant yeast *Kluyveromyces marxianus* as a microbial host for volatile ester biosynthesis. **A. Loebs**, C.M. Schwartz, I.R. Wheeldon

4:00 BIOT 550. Global metabolic rewiring for 2,3-butanediol production in cyanobacteria. **A. Carroll**, M. Kanno, N. Nozzi, A. Case, S. Atsumi

4:20 BIOT 551. Synthetic biology tools for the purple, non-sulfur bacterium *Rhodopseudomonas palustris* CGA009. **C. Immethun**, X. He, R. Saha

4:40 BIOT 552. Designing a continuous perfusion process for manufacturing antimicrobial peptides in *Drosophila melanogaster* S2 cells. **T. Weidner**, J. Zitzmann, D. Salzig, P. Czermak

Section C
InterContinental New Orleans
Pelican I/II

End-to-End Biomanufacturing

Disruptive Bioprocessing & Process Integration

S.W. Harcum, V. Natarajan, N. Rathore, S.A. Tobler, *Organizers*
A. Hewig, M. Westoby, *Presiding*

2:00 BIOT 553. Continuous manufacture of biopharmaceuticals: Engineering solutions to enable improved productivity and facility capacity management. **J. Pezzini**

2:20 BIOT 554. Quantitative assessment of environmental impact of biologics manufacturing using process mass intensity (PMI) analysis. S. Madabhushi, **J. Gavin**, S. Xu, C. Cutler, R. Chmielowski, W. Rayfield, N. Tugcu, H. Chen

2:40 BIOT 555. Pall Cadence Acoustic Separator for continuous perfusion cell culture: Cell retention device and downstream filtration. **K. Galipeau**

3:00 BIOT 556. Demonstrating viral clearance for a novel approach to continuous viral filtration. **T. Vetter**, M.J. Coolbaugh, V. Warikoo, K. Brower

3:20 Intermission.

3:40 BIOT 557. Can integrated continuous processing occur at the 12kL scale? **J.L. Coffman**, H. Lin, J. Salm, G. Hiller, S. Godfrey, S. Wang, R. Fahrner, R. Kottmeier, R. Orozco, S.S. Yildirim, D. Sullivan

4:00 BIOT 558. Viral clearance validation across continuous capture chromatography. **S. Chollangi**, J.M. Angelo, X. Xu, S. Ghose, M. Morbidelli

4:20 BIOT 559. Eliminating architectural segregation of pre and post viral manufacturing suites. **P. Clark**

4:40 BIOT 560. General platform for development of integrated downstream processes. **B. Nilsson**, A. Löfgren, J.F. Gomis, N. Andersson, L. Berghard, P. Tiainen, A. Staby

Section D
InterContinental New Orleans
Frenchman Ballroom

Biomedical & Emerging Technologies

Disease & Biomedical Applications

A.M. Kloxin, A. Noyes, J.P. Pieracci, *Organizers*
A. Berrill, S.L. Servoss, H.D. Sikes, *Presiding*

2:00 BIOT 561. Differences in antibody transport at the human blood-brain barrier. **J. Ruano-Salguero**, K. Lee

2:20 BIOT 562. EXO-TIP: A novel immuno-photolytic method for the isolation of highly purified neuronal exosomes. **M. Alam**, T. Bilousova, J. Campagna, V. John

2:40 BIOT 563. Inhibition of bacterial toxin activity using receptor-based peptides. E. Krueger, E. Koufos, **A.C. Brown**

3:00 BIOT 564. New myeloperoxidase detection system based on enzyme-catalysed dye oxidative polymerization for paper-based diagnostic device. **A. Bassegoda**, G. Ferreres, S. Perez Rafael, T. Tzanov

3:20 Intermission.

3:40 BIOT 565. Fluid shear stress as a circulating tumor cell model for testing chemotherapy drug resistance in breast cancer cell lines. **U.L. Triantafillu**, Y. Kim

4:00 BIOT 566. Investigating H_2O_2-induced cell death using a tunable, localized generator of peroxide in mammalian cell mitochondria. **K. Stein**, H. Sikes

4:20 BIOT 567. Investigating how physicochemical properties of extracellular matrix influence apparent diffusion coefficient in MRI. **H. Macdonald**, J. Bamber, M. Ryadnov, D. Collins, M. Rata, N. deSouza

4:40 BIOT 568. Modeling diseased blood-brain barrier utilizing patient-derived iPSCs and potential for rescue via amphiphilic block copolymer treatment. **H. Seo**, C. Lee, F. Bates, J. Tolar, S. Azarin

BIOL

Division of Biological Chemistry

S. Kelley, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Advances in Molecular Recognition of Double-Helical DNA & RNA (see *CARB*, Mon, Tue)

Discovery of Small Molecules Targeting RNA: Where Are We & Where Are We Going? (see *MEDI*, Wed)

Discovery of Small Molecules Targeting RNA (see *ORGN*, Tue)

Biologically Related Molecules & Processes (see *ORGN*, Sun, Mon, Tue)

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 243

Enzymes in Natural Product Biosynthesis Pathways

S.O. Kelley, *Organizer*
A.K. Boal, *Organizer, Presiding*

9:00 BIOL 1. Radical SAM enzymes in the biosynthesis of sugar-containing natural products. **H. Liu**

9:40 BIOL 2. X-ray crystallographic characterization of the reaction cycle in an iron(II) and 2-(oxo)-glutarate-dependent oxygenase. **A. Boal**

10:20 Intermission.

10:35 BIOL 3. Discovering unusual enzymatic chemistry in the microbial world. **E.P. Balskus**

11:15 BIOL 4. Complexity generation in the biosynthesis of fungal polyketide-nonribosomal peptide natural products. **Y. Tang**

Section B
Ernest N. Morial Convention Center
Room 244

Graduate Student & Postdoctoral Fellow Symposium

S.O. Kelley, *Organizer*
P.C. Bevilacqua, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 BIOL 5. Electric field optimization in enzymes. **V. Vaissier**, A. Bhowmick, S.C. Sharma, K. Schaettle, T.L. Head-Gordon

8:50 BIOL 6. C-terminal 'tail' of *M. tuberculosis* acyl carrier protein, AcpM, is provides a second mode of substrate sequestration for (very) long fatty acyl chains. **A. Patel**, K. Finzel, D. Lee, J. McCammon

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9:05 BIOL 7. Hydration at the protein surface: Observations from high-resolution data. **J.C. Miner**, J. Berendzen, P. Fenimore

9:20 BIOL 8. Probing ion-dependent changes to calmodulin binding site conformation with FTIR and ultrafast 2DIR spectroscopy. **S.C. Edington**, A. Gonzalez, T.R. Middendorf, D.B. Halling, R.W. Aldrich, C.R. Baiz

9:35 BIOL 9. Enzyme stabilization via computationally guided protein stapling. **E. Moore**, R. Fasan

9:50 BIOL 10. Internal mechanics of PPIP5K, a versatile molecular machine. **Y. An**, H. Wang, S. Shears, D. Kireev

10:05 Intermission.

10:20 BIOL 11. Elusive labile iron: Bioanalytical techniques to measure iron speciation in human plasma. **H.M. Neu**, S.A. Alexishin, J.E. Brandis, A.M. Williams, D. Sun, N. Zheng, W. Jian, J.E. Polli, M.A. Kane, S.L. Michel

10:35 BIOL 12. Small molecule potentiation of Gram-positive selective antibiotics against Gram-negative *Acinetobacter baumannii*. **S.E. Martin**, C. Melander

10:50 BIOL 13. Elucidation of drug-drug interactions at the transcriptional level in hepatocytes. **B. Bulutoglu**, C. Rey Bedon, S. Mert, O. Usta, M. Yarmush

11:05 BIOL 14. Design of a programmable and tunable semi-synthetic "clot buster". **P. Mukherjee**, L.J. Leman, J. Griffin, M. Ghadiri

11:20 BIOL 15. Withdrawn

11:35 BIOL 16. Nonenzymatic and chemoselective synthesis of ceramides in living cells. **A.K. Rudd**, N.K. Devaraj

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Biomineralization & Bio-Compatible Minerals
Sponsored by GEOC, Cosponsored by BIOL and ENVR

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 243

RNA Structure and Function

P.C. Bevilacqua, S.O. Kelley, *Organizers*
P. Bevilacqua, *Presiding*

1:00 BIOL 17. Catalytic strategies of small ribozymes from comparative analysis of active sites. **P.C. Bevilacqua**, D. Seith, J. Bingaman, A.J. Veenis, A. Button

1:35 BIOL 18. Secondary structure stability favors RNA thermostability under cellular conditions in a functional RNA. **K. Leamy**, N. Yennawar, P. Bevilacqua

1:55 BIOL 19. Emergence of ribonuclease activity in ribozymes through intersection of neutral networks. **J.A. Piccirilli**

2:30 BIOL 20. Probing general acid-base catalysis in Varkud satellite ribozyme with minimally perturbative nucleobase analogs. **B. Weissman**, N. Li, J.A. Piccirilli

2:50 Intermission.

3:10 BIOL 21. Kinetic isotope effect analyses of the transitionn states of non-enzymatic RNA 2′-*O*-transphosphorylation reactions catalyzed by acid, base and metal ions: Implications for biological catalysis. **M. Harris**

3:45 BIOL 22. Kinetic isotope effects on catalysis by the HDV ribozyme- precise determination of isotope ratios using electrospray ionization time-of-flight mass spectrometry. **H. Lin**, B. Weissman, S. Gardezi, V. Anderson, D.M. York, J.A. Piccirilli, M. Harris

4:05 BIOL 23. Insights into the diverse array of catalytic strategies of RNA enzymes from computational enzymology. **D.M. York**

4:40 BIOL 24. Computational RNA enzymology: Unravelling the catalytic mechanism of the twister ribozyme. **C.S. Gaines**, D.M. York

Section B
Ernest N. Morial Convention Center
Room 244

Chemical Tools for Modulating and Imaging Biology

M.E. Farkas, *Organizer, Presiding*

1:30 BIOL 25. Chemical tools for probing, manipulating, and imaging biological systems in space and time. **D.M. Chenoweth**

2:00 BIOL 26. Chemical modulation of circadian rhythms for the study of cancer. **M.E. Farkas**

2:30 BIOL 27. Modulating the immune response: Probing a code without a key. **A.P. Esser-Kahn**

3:00 Intermission.

3:15 BIOL 28. Sensing patterns in RNA structure and recognition via small molecules. C.S. Eubanks, B. Zhao, Q. Zhang, **A.E. Hargrove**

3:45 BIOL 29. Tools for visualizing and manipulating lipid signaling. **C. Schultz**

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Biomineralization & Bio-Compatible Minerals
Sponsored by GEOC, Cosponsored by BIOL and ENVR

SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall E

Current Topics

P.C. Bevilacqua, S.O. Kelley, *Organizers*

7:00–9:00

BIOL 30. Lipid membrane formation in artificial cells. **J. Flores**, H. Niederholtmeyer, A. Bhattacharya, N.K. Devaraj

BIOL 31. Direct detection of xanthurenate radical from enzymatic oxidation of xanthurenic acid. **B.E. Sturgeon**, C. Folluo, C. Knutson, A. Motten, R.P. Mason, J.E. Roberts

BIOL 32. The pattern of occurrence of cytosine in the genetic code. **B. Wang**

BIOL 33. Analyzing the role of G●U base pairs on the melting behavior of the *S. enterica htrA* RNA thermometer. **E.K. Choi**, R.M. Mitton-Fry

BIOL 34. Expression and characterization of dehydrogenase domain of NADPH oxidase 5. **J. Iverson**, E. Hay, C. Wei

BIOL 35. Withdrawn

BIOL 36. Optimizing methods for analyzing O-GlcNAc modifications. **M. Navarro**, A. Batt, K.N. Chuh, M. Pratt

BIOL 37. Structural and solution studies of DNA-binding by SloR, A Mn-dependent regulatory protein from *Streptococcus mutans*. S. Bender, G. Spatafora, J.Z. Chen, **A. Glasfeld**

BIOL 38. Synthetic α-helix mimetics for recognition of HIV TAR-RNA. **D. Maity**, S. Kumar, A.D. Hamilton

BIOL 39. Refractive index matching mounting media for best-in-class sample preservation and image quality. **A.W. York**, D. Cash, B. Boal, O. Golub, M. Wickman, E. Welch

BIOL 40. Synthesis and screening of a β amino acid bisintercalator library. **E. Gratton**, B.L. Iverson

BIOL 41. Addition of backbone modified amino acids to mRNA display via an editing-deficient aminoacyl-tRNA synthetase. **E.S. Iqbal**

BIOL 42. Engineering a replicative DNA polymerase for accurate bypass of damaged DNA. **T. Coulther**, M.J. Ondrechen, P.J. Beuning

BIOL 43. Site-directed mutagenesis of rSERT in preparation for future crosslinking studies. **H. Gering**, E. Costellano, M. Cascio

BIOL 44. DNA patterning methods for the study of a designed bacterial community. **M.J. Smith**, A. Furst, M.B. Francis

BIOL 45. Construction of synthetic membranes by chemoselective lipidation of peptides. **C.J. Cho**

BIOL 46. Testing the limits of NO detection with liposome encapsulated spin trap. V. Akkaraju, R. Diao, B. Schieler, K. Bidle, **D.J. Hirsh**

BIOL 47. Mechanism of triazolium salts on breast cancer cells. **J.J. Bies**, Z. Lin, K. Taylor, J. Meyers

BIOL 48. Catalysis of transthioacylation in the active centers of dihydrolipoamide acyltransacetylase components of 2-oxo acid dehydrogenase complexes: A reassessment of mechanism. **J. Chakraborty**, N.S. Nemeria, E.T. Farinas, F. Jordan

BIOL 49. Careful what you label for: A Story of peril and intrigue in fluorophore labeling for tracking cellular uptake. **J.M. Larson**, A.P. Blum, H. Conteh

BIOL 50. DNA:RNA hetero-guanine quadruplex formation: Duplex guidance and disruption by peptide nucleic acid. **A. Berlyoung**, B.A. Armitage

BIOL 51. Modular biotinylated and photoactive NAADP analogs. **Y. Zhang**, J. Slama, T. Walseth

BIOL 52. Characterization of a small molecule's influence on a Ras-related protein-protein interaction. **A. Montoya-Beltran**, P.D. Adams

BIOL 53. *RNA-seq* analysis of *Komagataeibacter xylinus* E25 A:kan and AB::kan mutants. **P. Jacek**

BIOL 54. Inhibition of amyloid fibril formation via naturally occuring phenolic compounds monitored by atomic force microscopy. **C. Pollock**, D. Dasani, T. Nghiem, R. Vitale, **D.F. Moriarty**

BIOL 55. Isolation and characterization of antibacterial molecules from various fruits and spices. **A. Smith**, S. Jones, M. Khan, **D.F. Moriarty**

BIOL 56. Coiled-coil peptides: A template for investigating connection between stability and sequences. E. Allgeyer, W. Cross, P. Fisk, **M. Blackburn**

BIOL 57. Controlled microbial biosynthesis of Cd and Zn quantum dots. **S. Lampa-Pastirk**, S. Forney, A.M. Bell

BIOL 58. Conserved aromatic residues at the dimer-dimer interface in the yeast peroxiredoxin Tsa1 facilitate decamer formation and biological function. M.A. Loberg, J.E. Hurtig, A.H. Graff, K.M. Allan, J.A. Buchan, M.K. Spencer, J.E. Kelly, J.E. Clodfelter, K.A. Morano, W. Lowther, **J.D. West**

BIOL 59. Structure-activity relationships for activation of *Arabidopsis thaliana* cytokinin receptors by analogs of N^6-benzyladenine. **D.I. Osolodkin**, E. Savelieva, D. Karlov, V. Oslovsky, S. Lomin, S.N. Mikhailov, G. Romanov

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BIOL 60. Direct ESR detection of lignin monomer radicals. **S. Saey**, Z.A. Taylor, B.E. Sturgeon

BIOL 61. A possible mechanism of turmeric anti-cancer activity. **K.M. Counter**, J.J. Parackal, R. Sheaff

BIOL 62. Effects of familial mutations on the structure and assembly of a peptide derived from $A\beta_{16-36}$. **K.J. McKnelly**, S. Yoo, A. Kreutzer, J.S. Nowick

BIOL 63. Toward the detection of cancers by chemotaxis of *C. elegans*. **E.J. Eggers**

BIOL 64. Elucidating the role of the sRNA C.0293 in the bacterial stress response. **R.E. Miner**, A. Sehgal, M. Popek, J. Pellino

BIOL 65. Stable binding of protein RsmG to 16S helix 18 requires RNA-protein and RNA-RNA contacts formed by the 16S 5′-domain RNA. **C.M. Hawkins**, S. Abeysirigunawardena

BIOL 66. Mutational analysis of A2-domain interface residues in promoting the structural stability of blood coagulation factor vIIIa: A computational binding free-energy analysis study. **D. Venkateswarlu**, S. Shearin

BIOL 67. Revisiting the acetaminophen free radical. **B.C. Stillwell**, I.C. Salveson, J.K. Ricketts-Hagan, B.E. Sturgeon

BIOL 68. Withdrawn

BIOL 69. High throughput *in vivo* screening assay for novel inhibitors of extracellular heme sensing and utilization in *Pseudomonas aeruginosa*. **E. Robinson**, D. Liang, S. Mouriño, F. Xue, A. Wilks

BIOL 70. The preliminary study of hOLA1 N-terminal methylation catalyzed by NRMT1. **J. Burgos Rivera**, K. Jia, P. Li

BIOL 71. Evaluation and biophysical characterization of novel antimicrobial peptides: "A water purification approach". **V. Ortiz Gomez**, V. Rodriguez, E. Nicolau

BIOL 72. Human skin RNases offer dual protection against invading bacteria. **B. Wang**

BIOL 73. Net1A inhibitors: Looking for synergy. **M. Jones**, A. Ulu, Y. Zuo, J.A. Frost

BIOL 74. Phosphorylation and regulation of the splicing factor SRSF1 by a symbiotic kinase-kinase SRPK1-CLK1 complex. **B. Aubol**, J. Adams

BIOL 75. Self-assembly and photophysical characterization of synthetically functionalized luciferins for detecting host-guest interactions. **H.P. Rahn**, E.B. Atuk, J. Jayawickramarajah

BIOL 76. Evaluation of mosquito (*A. aegypti*) organic anion transporters through microinjection of sulfuryl group dyes. **B. NIcholls**, M. Rouhier

BIOL 77. Enzymatic synthesis of endocannabinoids. **S.L. Weber**, R.M. Hyslop, P.D. Burns

BIOL 78. Base composition and sequence characteristics of the 5′UTR of BACE1 mRNA. **B. Wang**, D. Lycans

BIOL 79. Design of new natural cysteine protease inhibitors (CPI) in complex with cruzipain from *T. cruzi*. **R. Espinosa**, A. Juarez-Saldivar, G. Rivera

BIOL 80. A synthetic isoprenoid lipoquinone, menaquinone-2, adopts a folded conformation in solution and at a model membrane interface. **D.C. Crans**, J.T. Koehn, E.S. Magallanes, B.J. Peters, C.N. Beuning, A.A. Haase, M.J. Zhu, C.D. Rithner, D.C. Crick

BIOL 81. Perturbing the BfrB:Bfd interaction of *Pseudomonas aeruginosa* by chemical and genetic intervention causes irreversible accumulation of iron in BfrB. **A. Punchi Hewage**, H. Yao, K.K. Gnanasekaran, M.M. Lee, S. Phaniraj, S. Lovell, R.A. Bunce, B.R. Peterson, M.E. Rivera

BIOL 82. Structural changes of chloroplast signal recognition particle proteins studied by single molecule FRET during vectorial protein targeting. **D. Baucom**, R. Hendersen, R. Goforth, A. Kight, P. Sharma, F. Gao, S. Kumar, R.L. Henry, C.D. Heyes

BIOL 83. Assessing apoptosis inducing factor (AIF) as a candidate tumor promoter. **S. Birua**

BIOL 84. Designing peptide inhibitors for annihilating amyloid deposits: Treating Alzheimer's disease. **P. Prasad**, S. Chakraborty

BIOL 85. Cannabinoids as anti-cancer agents: What's really going on? **J.A. Folsom**, N. Pullen, C.E. Brown, R.M. Hyslop, P.D. Burns

BIOL 86. Arylboronic acid-catalyzed hydrolysis of salicylaldehyde imines mimics Michaelis-Menten enzyme-substrate kinetics. **C.C. Clement**, M. Philipp, S. Zakia

BIOL 87. Design, synthesis, molecular docking and antimicrobial activity of New 7-(4-(2-((1,2,4-triazol-3-yl)thio) acetyl)piperazin-1-yl) derivatives of ciprofloxacin. H.H. Mohammed, **E.M. Abdelhafez**, S.H. Abbas, G.A. Abuo-Rahma, G. Hauk, J.M. Berger, S. Mitarai, M. Arai, K.N. Dalby, **T.S. Kaoud**

BIOL 88. Cannabidiol dimethyl ether synthesis pathways. **T. Cale**, R.M. Hyslop, C.E. Brown, S. Bydalek

BIOL 89. Triacylglycerols play a protective role during apoptosis. **N. Li**, G. Atilla-Gokcumen

BIOL 90. Development of a chemical proteomic strategy to target diacylglycerol kinases. **C.E. Franks**, S.T. Campbell, B.W. Purow, T.E. Harris, K. Hsu

BIOL 91. Stability of nonproteinogenic amino acids under extraterrestrial conditions. **L.A. Rowe**, J.R. Peller, C.C. Mammoser, K. Davidson, S. Dhar, A.J. Gunter, G. Burkhart, B. Brown

BIOL 92. Amyloid diversity in yeast is promoted by prion-specific chaperone functions. **J.K. Hines**

BIOL 93. NADPH-dependent reductive aminases. **M. Sharma**

BIOL 94. Aromatic ynamines: A new bio-orthogonal reactive group for step-efficient, sequential bioconjugation. **M. Hatit**, A.J. Watson, G.A. Burley

BIOL 95. Patronage of chemical safety and security among chemistry professionals. **E.O. Nwaichi**, T. Salah

BIOL 96. Progression towards structural determination and the understanding of protein-protein interactions of terminin complex proteins. **E.M. Miller**, C. Brazel, M. Loncaric, G. Horner, K. Kuznacic, A. Neibert, R. Kurzhals, C. Ragain

BIOL 97. Synthesis and characterization of biogenic selenium nanoparticles with antimicrobial properties made by *Staphylococcus aureus*, Methicillin-resistant *Staphylococcus aureus* (MRSA), *Escherichia coli* and *Pseudomonas aeruginosa*. **D. Medina Cruz**, T. Webster, A. Roy

BIOL 98. Short cationic peptides induce pH-sensitive non-leaky membrane fusion to enable cytoplasmic delivery of cell-impermeable compounds. L. Hui, F. Wang, L. Xu, F. Gao, Z. Zhao, **L. Yang**

BIOL 99. Prevention and treatment of oral gonorrhea using antimicrobial GUMBOS. **K.M. Lopez**, M. Cole, J. Hobden, I.M. Warner

BIOL 100. Nanosized calcium-responsive contrast agents for functional MRI applications. **G. Gambino**, T. Savić, G. Angelovski

BIOL 101. "Geometric mutation" for decoupling receptor signaling crosstalk at phagosome membranes. **W. Li**, Y. Yu

BIOL 102. Effect of substrate presentation and Michaelis complex stability on neuraminidase 2 (NEU2) specificity. O.C. Grant, S. Makeneni, B.L. Foley, **R.J. Woods**

BIOL 103. Unexpected binding specificity of 2OST: Implications for heparan sulfate biosynthesis. D.F. Thieker, J. Liu, Y. Xu, C. Nora, J. Esko, H. Qiu, L. Wang, **R.J. Woods**

BIOL 104. Polyacrylamide nanoparticles: A conjugatable platform for use in the diagnosis and treatment of cancer. **S. Yap**, G. Stasiuk, R. Boyle

BIOL 105. Biochemistry of clinically relevant ITPase mutants. **N.E. Burgis**

BIOL 106. QM-cluster model examination of a biphenyl transition state "trapped" within an engineered Thr-tRNA synthetase. **T.J. Summers**, Q. Cheng, N.J. Deyonker

BIOL 107. Interactions of platinum(II) small molecules with RNA and implications of platination on RNA depurination and cell cytotoxicity. **B. Kimutai**

BIOL 108. Withdrawn

BIOL 109. The small molecule 2-Azido-2-deoxy-glucose is a metabolic chemical reporter of O-GlcNAc modifications in mammalian cells, revealing an unexpected promiscuity of O-GlcNAc transferase. **A. Batt**, B. Zaro, K.N. Chuh, M. Navarro, M. Pratt

BIOL 110. Mechanistic study of a peptide diastereomer with anti-cancer activity. **J. Yu**, T.B. Shrestha, A.I. Herreira, O. Prakash, D.L. Troyer, S.H. Bossmann

BIOL 111. Real-time ticking of a biological clock, assembled in a test tube. **J. Heisler**, Y. Chang, A. Chavan, A. LiWang

BIOL 112. Mechanistic insights into oligomer and fibril formation of amyloid-beta peptide. **D. Du**

BIOL 113. An NMR based metabolomics approach to understanding biochar's effects on *Escherichia coli*. **R. Hill**, **A.H. Byers**, J. Hunt, E. Sanders, T. MIsna, N. Fitzkee

BIOL 114. Pin1-histone H1 interactions: Towards an understanding of substrate specific activity. **D. Jinasena**, H. Gyamfi

BIOL 115. Mechanistic studies of copper-activated drugs against Gram-positive bacteria. **M. Kalubowilage**, A. Delpe Acharige, M. Zhang, A.P. Malalasekera, F. Wolschendorf, S.H. Bossmann

BIOL 116. Flow cytometry based high-throughput screen capable of sorting biofuel producing *E. coli* cells. **J. Freeman**

BIOL 117. Probing the effects of oligomerization and heme pocket residues on the signal transduction within globin coupled sensors. **S. Rivera**, E.E. Weinert

BIOL 118. Mechanism of a class C radical SAM thiazole methyltransferase. **N. Mahanta**, Z. Zhang, G.A. Hudson, W.A. Van Der Donk, D. Mitchell

BIOL 119. Nano structure design for RNA interference. **Z. Shu**, N. Abe, F. Tomoike, Y. Kimura, Y. Ito, H. Abe

BIOL 120. Cellular effects of ligand binding to the Oxysterol-binding protein family (OSBP/ORP4). **B. Roberts**, Z. Severance, R. Bensen, N.R. Kothapalli, J.I. Nunez, H. Ma, S. Wu, A. Burgett

BIOL 121. Selective peptide binders for PDL1 as an immunogenic target in cancer. **G. Kamalinia**, T. Takahashi, R.W. Roberts

BIOL 122. Peptidomimetic inhibitors of the KDM4-subfamily of histone lysine demethylases: Transitioning from substrate to inhibitor. **J. Maw**, Y. Le Bihan, K. Tomlin, N. Mok, V. Bavetsias, J. Blagg

BIOL 123. Withdrawn

BIOL 124. Automated and high-resolution force spectroscopy for biochemical applications. **H. Jia**, S. Xu

BIOL 125. Force-selected molecular printing with high precision and versatility. **Y. Mao**, Q. Hu, S. Xu

BIOL 126. Isolation and characterization of a novel intermediate of thymidylate synthase: Possibility of a new class of chemotherapeutic drugs targeting thymidylate synthase. **A.K. Ghosh**, S. Kholodar, A. Kohen

BIOL 127. Functional analysis of O-GlcNAc modified β-synuclein using synthetic protein chemistry. **A. Galesic**, P. Levine, A.J. Balana, M. Pratt

BIOL 128. Withdrawn

BIOL 129. Human serum albumin is conformationally changed in the presence of epigallocatechin gallate using FRET

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(Förster resonance energy transfer). **X. Sun**, A.E. Hagerman

BIOL 130. Trehalose monomycolate mimic chemical reporter: A strategy for detecting, profiling and identifying O-mycoloylated proteins in mycobacterium. **H.W. Kavunja**, B. Piligian, T. Fiolek, H. Foley, T. Nathan, B.M. Swarts

BIOL 131. 6-Thiopurine: Targeting UDP-glucose dehydrogenase and its efficacy effects. **C.J. Weeramange**, R.J. Rafferty

BIOL 132. Synthesis and application of small molecule probes for lipid labeling. **A.J. Carr**, S. Alam, T.J. Ricks, X. Zhang, M. Best

BIOL 133. Withdrawn

BIOL 134. FRET based assays to study the binding of fibroblast growth factor to its receptor. **M. Mohale**, A. Howard, M. Crew, S. Jayanthi, S.K. Thallapuranam, C.D. Heyes

BIOL 135. A beacon in the night: Chemiluminescence imaging agents for whole animal imaging. **A.R. Lippert**

BIOL 136. Distinct immune responses with covalently-linked TLR agonist combinations for a Q-Fever vaccine. **T.J. Albin**, J. Tom, S. Manna, A. Gilkes, M. Supnet, H. Davies, A. Jain, R. Nakajima, A. Jasinskas, S. Ruiz, A. Nalca, A. Burkhardt, P. Felgner, A.P. Esser-Kahn

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 243

Ralph F. Hirschmann Award in Peptide Chemistry: Symposium in honor of Lila M. Gierasch

Bridging Peptides & Proteins: From Function to Therapy

Cosponsored by WCC
Financially supported by Journal of Biological Chemistry and University of Massachsetts Amherst
L.M. Gierasch, S.O. Kelley, *Organizers*
J.P. Schneider, *Presiding*

9:00 Introductory Remarks.

9:10 BIOL 137. Conformational imprinting and amyloid disease. **S. Radford**

9:40 Intermission.

9:45 BIOL 138. Racemic hydrogels from self-assembling mirror image peptides: Predictions from Pauling and Corey. **J.P. Schneider**

10:15 Intermission.

10:20 BIOL 139. Designed FN3 Domains for extrahepatic delivery of oligonucleotides. **K. ONeil**

10:50 Intermission.

10:55 BIOL 140. Molecular interactions between collagen and its binding partners: access to cryptic binding sites. **J. Baum**, D. Case, C. Hoop, A. Kemraj, A. Nunes, J. Zhu

11:25 Intermission.
11:30 BIOL 141. Award Address
(Ralph F. Hirschmann Award in Peptide Chemistry Sponsored by the Merck Research Laboratories). When peptides mimic proteins, and when they do not: Promiscuous selectivity in Hsp70 chaperone binding of substrates. E.M. Clerico, C.A. English, J.M. Tilitsky, W. Meng, J. Chen, W. Sherman, **L.M. Gierasch**

Section B
Ernest N. Morial Convention Center
Room 244

Chemical Tools for Interrogating Biological Systems

S.O. Kelley, *Organizer*
C.I. Stains, *Organizer, Presiding*

8:30 BIOL 142. New fluorophore scaffolds for chemical biology. **C.I. Stains**

9:05 BIOL 143. Engineered protein switches for controlling dynamic cellular processes. **D.J. Maly**

9:40 BIOL 144. Protein engineering approaches for targeting and understanding protein kinases and phosphatases in live cells. **I. Ghosh**

10:15 Intermission.

10:25 BIOL 145. Spying on cellular communication with chemical probes and noninvasive imaging. **J.A. Prescher**

11:00 BIOL 146. Optical control of protein function through genetic code expansion in cells and animals. **A. Deiters**

11:35 BIOL 147. Activity-based sensing approaches to studying chemistry in living systems. **C.J. Chang**

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 243

Goodman Award Symposium

H. Crichton, S.O. Kelley, *Organizers*
W.F. Degrado, *Presiding*

1:30 Introductory Remarks.

1:35 BIOL 148. Inverse drug discovery. **J.W. Kelly**

2:05 BIOL 149. Domain cross-talk in epigenetic regulation. **D.G. Fujimori**

2:35 BIOL 150. Small molecule immunomodulators that target toll-like receptors. **H.H. Yin**

3:05 Intermission.

3:20 BIOL 151. Molecular mechanisms for atypical functions of protein kinases. **N. Jura**

3:50 BIOL 152. Minimalist design of peptide and protein catalysts. **I.V. Korendovych**

4:20 BIOL 153. De novo protein design. **W.F. Degrado**

Section B
Ernest N. Morial Convention Center
Room 244

Early Career Investigators in Biological Chemistry

P.C. Bevilacqua, *Organizer*
S.O. Kelley, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 BIOL 154. Viral hijacking of host proteins through fuzzy interactions: Mechanism and application. Q. Shen, J. Shi, D. Zeng, B. Zhao, P. Li, W. Hwang, **J. Cho**

1:55 BIOL 155. Biosynthesis of beta-lactones. **T.A. Wencewicz**

2:15 BIOL 156. Light in sound out: Development of acoustogenic probes for *in vivo* imaging of reactive nitrogen species. **J. Chan**, C.J. Reinhardt, E. Zhou

2:35 BIOL 157. Optical imaging tools for elucidating the roles of anions in cellular signaling. **S. Dodani**

2:55 BIOL 158. Chemoproteomic discovery of lipid kinase inhibitors for immuno-oncology. **K. Hsu**

3:15 Intermission.

3:30 BIOL 159. Cell-specific chemical libraries targeting immune supression in the tumor microenvironment. E. Kischuk, J. Majumder, J. Fine, T. Lantz, D. Dhawan, D. Knapp, T. Ratliff, **G. Chopra**

3:50 BIOL 160. Mirror image aptamers and ribozymes: Targeting RNA through heterochiral nucleic acid interactions. **J.T. Sczepanski**

4:10 BIOL 161. Chemical probes for monitoring interactions between reactive sulfur, oxygen, and nitrogen species in the airways of human subjects. **A.R. Lippert**

4:30 BIOL 162. Novel activity-based chemical probes for human sirtuins. E. Graham, S. Rymarchyk, S. Zheng, **Y. Cen**

4:50 BIOL 163. Chemical ligation reaction for oligonucleotides based on electrophilic phosphorothioester. **Y. Kimura**, H. Maruyama, R. Oikawa, M. Hayakawa, N. Abe, G. Tsuji, A. Matsuda, S. Shuto, Y. Ito, H. Abe

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix

S.O. Kelley, *Organizer*

8:00–10:00

30, 38, 44, 54, 80. See previous listings.

179, 181, 189-191, 194, 197, 199-200, 205, 209, 228-229, 241, 249. See subsequent listings.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 243

ACS Chemical Biology Award Symposium

S.O. Kelley, A. Weidmann, *Organizers*
L.L. Kiessling, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 BIOL 164. Deciphering the human microbiota with chemistry. **E.P. Balskus**

9:35 BIOL 165. Chemical editing of the glycocalyx to influence cellular functions. **K. Godula**

10:05 BIOL 166. Mighty chemistry of bacterial small molecules. **B. Li**

10:35 BIOL 167. Olfactory receptor-based sensors to accelerate the engineering of chemical-producing microbes. **P. Peralta Yahya**

11:05 Introduction of Awardee.

11:10 BIOL 168. Detecting and attacking cancer surface-omes with recombinant antibodies. **J.A. Wells**

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

Chemists & Writing for Fun & Profit: Write Your Own Career
Sponsored by SCHB, Cosponsored by BIOL and PROF

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 243

Ronald Breslow Award for Achievement in Biomimetic Chemistry: Symposium in honor of David R. Liu

S.O. Kelley, *Organizer*
D.R. Liu, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 BIOL 169. Chemical biology-based approach to understanding and overcoming cancer therapy resistance.

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S.L. Schreiber

2:20 BIOL 170. Life 2.0: Synthetic self-replicating and evolving systems. **G.F. Joyce**

3:05 Intermission.

3:20 BIOL 171. Playing with the Molecules of Life. **P.G. Schultz**

4:05 BIOL 172. Award Address (Ronald Breslow Award for Achievement in Biomimetic Chemistry Sponsored by the Ronald Breslow Award Endowment). Base editing: Chemistry on a target nucleotide in the genome of living cells. **D. Liu**

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall E

Current Topics

P.C. Bevilacqua, S.O. Kelley, *Organizers*

7:00–9:00

BIOL 173. Protein determinants of anion binding: Application to sodium iodide symporter. **H. Zhekova**, M. Damergi, X.Q. Lu, S. Gupta, C. Hsieh, S. Noskov

BIOL 174. Withdrawn

BIOL 175. Progress towards the structural determination of the telomere associating protein Modigliani. **C. Brazel**, E.M. Miller, G. Horner, M. Loncaric, K. Kuznacic, A. Neibert, R. Kurzhals, C. Ragain

BIOL 176. Design of a dimeric aptamer against B-cell receptor. **S. Batool**, H. Zumrut, S. Bhandari, N. Van, S. George, P. Mallikaratchy

BIOL 177. Role of CDKs on glioblastoma cell growth. **M. Palha**, R.H. Lee, Z. Bacugalupa, M. Reginato

BIOL 178. pH-dependent studies of the reductive half-reaction of methylenetetrahydrofolate reductase from *Escherichia coli*. **A. Li**, J. Wang, E.E. Trimmer

BIOL 179. Studies into the mechanism of propanediol dehydratase: A glycyl radical enzyme highly abundant in healthy human gut microbiomes. **B.J. Levin**, E.P. Balskus

BIOL 180. Role of cell-surface hemin receptors in the rapid uptake and photodynamic inactivation of staphylococci by Ga(III)-protoporphyrin IX. **A.V. Morales**

BIOL 181. Probing the protein-protein interactions in bacterial fatty acid biosynthesis: Applications in antibacterial agent development, and biofuel production. **K. Charov**, M.D. Burkart

BIOL 182. Targeted depalmitoylation of N-Ras for suppression of oncogenic signaling pathways. **H. Vora**

BIOL 183. Correlating bacterial diversity to nitrogen contamination of alluvial aquifers in Iowa. **K. Miner**, C.L. Just

BIOL 184. Thiophene-*N*-methylbenzimidazole β–hole module as a new road to specific recognition of mixed DNA sequences. **P. Guo**, A. Paul, A. Kumar, A.A. Farahat, N. Harika, S. Wang, D.W. Boykin, W. Wilson

BIOL 185. New photoaffinity labeling module. **B. Zhao**, J. Taechalertpaisarn, K. Burgess

BIOL 186. Tissue-specific loss of SMN and its effect on the immune response of *Drosophila melanogaster*. **H.N. Dinh**, G. Matera, A. Spring, D. Brown

BIOL 187. Cloning and expression of recombinant chondroitinase AC II and its comparison to the *Arthrobacter auescens* enzyme. **A. Williams**, R.J. Linhardt, M. Koffas, B. Cress, W. He, T. Toida

BIOL 188. First structure of a designed minor groove binding heterocyclic cation that specifically recognizes mixed DNA base pair sequences. **N. Harika**, M.W. Germann, A. Paul, D.W. Boykin, W. Wilson

BIOL 189. Approaching the color problem of bioluminescence: Contributions of the active site microenvironment to the emission of red and green luciferases. **N. Lui**, C. Carrasco-López, J.C. Ferreria, S. Schramm, P. Naumov, W. Rabeh

BIOL 190. Biophysical approach to convert an "undruggable" DNA target to a "druggable" receptor. **A. Paul**, P. Guo, N. Harika, A. Kumar, A.A. Farahat, S. Laughlin, G.M. Poon, D.W. Boykin, W. Wilson

BIOL 191. Triazabutadiene drug conjugates for the identification of protein-protein interactions. **A. Shepard**, J.C. Jewett

BIOL 192. Y-FAST as a fluorescent color switchable reporter in living cells. **J. Kim**, H. Lee, H. Chung, H. Lee

BIOL 193. Investigating plasmid DNA maintenance in transformed E. coli. **T. Oh**, B. Hicks

BIOL 194. Functional characterization of GPCRs in synthetic membranes using *in situ* lipid synthesis for protein reconstitution technology. **K. Podolsky**, R.J. Brea, N.K. Devaraj

BIOL 195. Effects of the pro-cys-pro tripeptide stretch on the structural and biochemical properties of chloroperoxidase. **E. Kwong**, X. Wang

BIOL 196. Interaction of aurein 1.2 with vesicles mimicking normal and cancer cell membranes. **C.R. Alexander**, N. Phambu

BIOL 197. Investigating the binding mechanism between FMRP and Drosha mRNA G-quadruplex. **K. McDougal**, M. Mihailescu

BIOL 198. The effect of oxidative stress on mitochondrial electron transfer flavoprotein: Pinpointing sequences adducted by 4-hydroxy-2-nonenal. **E. Schaible**, **C.M. Byron**, D. Knapp, M. Breen-Lyles

BIOL 199. Mn^{2+}-sensing and conformational switching mechanism in the *Escherichia coli* Mn^{2+}-dependent riboswitch. **R. Cai**, I. Price, F. Ding, C. Lu, A. Ke

BIOL 200. Chemoproteomic methods for investigating mitochondrial cysteine oxidation in disease. **M. Pizzagalli**, D. Bak, E. Weerapana

BIOL 201. Regulatory mechanism of nitric oxide synthase by cav-1 and calmodulin. **N. Schimp**, C. Wei

BIOL 202. Characterization of the 3rd and 4th EF-hand motifs of NADPH oxidase 5 by calorimetry. **E. Fabry**, L. Lloyd, C. Wei

BIOL 203. Fullmetal alchemy: Using kinetic isotope effects to interrogate divalent metal ion catalysis in phosphoryl transfer enzymes. **E.W. Ollie**, J.A. Piccirilli, D.M. York, M. Harris

BIOL 204. Novel phosphinate-based near-infrared fluorophores and their biological application. **Y. Fang**, X. Zhou, C.I. Stains

BIOL 205. Advancing polymerase ribozymes towards self-replication. **K. Tjhung**, G.F. Joyce

BIOL 206. New views of head-to-middle prenyltransferases. **L. Chen**, J. Gao, S.R. Malwal, T. Kuo, M. Liu, W. Liu, Y. Yang, J. Huang, J. Zhang, F. Qu, C. Chen, Y. Zhang, R. Guo, E. Oldfield

BIOL 207. Induction of cell death mechanisms with light by a novel porphyrin derivative. **T.E. Hayes**, A. Abbott, H. Brandon, A. Savenka, A. Basnakian, J.E. Bradshaw

BIOL 208. Design and characterization of a dual-loop G-quadruplex for molecular logic gates. **C. Briney**, C.H. Battle

BIOL 209. Zinc influence on *Plasmodium falciparum* during intraerythrocytic development. **K. Payson**, E. Allman, M. Llinás

BIOL 210. Short dietary peptide IRW elicits its pharmacological effects via PGC1β axis. **K. Bhullar**, N. Pabon, C.J. Camacho, J. Wu

BIOL 211. Chemical reactive anchoring lipids with different performance for cell surface re-engineering. **M.L. Boron**, P. Vabbilisetty, H. Nie, E. Ozhegov, X. Sun

BIOL 212. Synthesis of diphosphate ProTides for enhancement of cellular metabolism. **M. de Cabrera**, S.F. Wnuk

BIOL 213. Creating dense DNA phases with protein-crosslinked plasmids. **C. Tsai**, N.K. Devaraj, H. Niederholtmeyer

BIOL 214. Cyanocarbazole derivatives as universal bases. **A. Shaver**, L.A. Truong, S.A. Woski

BIOL 215. Analysis of dopaminergic derivatives in sulfotransferase SULT1A3. **C. Cochrane**, D. Bigler, M.L. Cafiero, L.W. Peterson

BIOL 216. Investigating the conformational dynamics of GLP-1R: A class B G protein-coupled receptor. **T.M. Lewandowski-Baird**, C.P. Ramil, P. An, Q. Lin

BIOL 217. Augmenting vaccine immunogenicity through the use of natural human anti-Rha antibodies and monoclonal Fc domains. **M. Hossain**, A. Vartak, S. Sucheck, K. Wall

BIOL 218. Catalyzed reporter deposition for fluorescent labeling of cells using oxidative enzymes. **B.T. Cisneros**

BIOL 219. Metal binding affinity of *Halobacterium salinarum* cysteinyl-tRNA synthetase. **L. Cobani**, C.M. Evilia, J. Rosentreter, J. Kuhlmeier

BIOL 220. Withdrawn

BIOL 221. Dual targeted nanoparticles for mitochondrial delivery of a cisplatin prodrug for prostate cancer therapy. **B. Surnar**, S. Dhar

BIOL 222. LAT1 membrane transporter selectivity for L and D amino acids. **C. Hall**, **B. Venteicher**, H. Chien, K. Giacomini, C. Colas, A. Schlessinger, A.A. Thomas

BIOL 223. Role of serine to threonine substitution in NrdF protein of ribonucleotide reductase enzyme. M. Jayachandran, D. Cipurko, **O. Makhlynets**

BIOL 224. Design, synthesis and biological evaluation of novel NSAIDs with improved gastrointestinal safety profile. H.S. Abd-Ellah, A.M. Mohassab, M.E. Shoman, E.A. Beshr, H.A. Hassan, D. Abdelhamid, M. Abdel-Aziz, A.F. Ahmed, K.N. Dalby, **T.S. Kaoud**

BIOL 225. Chemical proteomic profiling of prenylated proteins involved in disease. **K.G. Suazo**, M.D. Distefano

BIOL 226. Microbiological aspects of energy production. **T. Komolafe**

BIOL 227. Liposomal delivery of diacylglycerol lipase-beta inhibitors to macrophages dramatically enhances selectivity and efficacy in vivo. **M. Shin**, H. Snyder, G. Donvito, L. Schurman, T. Fox, A. Lichtman, M. Kester, K. Hsu

BIOL 228. Targeting DNA methylation to enhance memory function. **A. Boitnott**, C.P. Gettens, X. Zhang, K. Zengeler, H. Smith, B. Malachowsky, A. Kennedy

BIOL 229. Spatiotemporal photo-regulation of translation by enzymatic covalent mRNA labeling. **D. Zhang**, E.C. Zhou, K.N. Busby, S.C. Alexander

BIOL 230. Synthesis, characterization and biological studies of cobalt(II) Schiff bases derived from o-vanillin with series of aromatic amines. **R.O. Shaibu**, G. Watkins

BIOL 231. PIP-on-a-chip assay: A microfluidics based approach to study viral protein – membrane interactions. **S.J. Sujansky**, C. Yeager, C.E. Cameron

BIOL 232. Mechanistic insights into quorum sensing regulator protein-DNA binding. **T.L. Schneider**, S. Durmus, R. Glasser

‡*Cooperative Cosponsorship*

BIOL 233. Toward development of protein-polymer conjugates for biocatalytic cyclopropanation. **H. Wu**, S. Onbulak, A. Sood, J. Rzayev, Q. Lin

BIOL 234. Increasing solubility of the serine protease dipeptidyl peptidase-4 via protein truncation. **S.F. Spradlin**, C.M. Evilia

BIOL 235. Design of a halophilic peptide based on halophilic protein motifs. **C. Brininger**, C.M. Evilia

BIOL 236. Elucidating the regulatory phosphorylation hotspots of full-length BRAF through enzymological analyses. **N. Cope**

BIOL 237. Identification of ssDNA aptamer specific to an herbicide. **K. Abraham**, K.L. Hong

BIOL 238. Investigating the roles of *Mycobacterium smegmatis* L,D-transpeptidases in cell wall biosynthesis. R.L. Marshburn, P.K. Stateler, T. Zandi, **L. Basta**

BIOL 239. Understanding the mechanism of mutation suppression by a conserved oxidant defense protein in yeast. **M. Pleshinger**, N.R. West, M.A. Loberg, J.B. David, B.A. Bauer, J.A. Buchan, T.J. Roston, K.M. Allan, I.C. Martin, S.R. Hohan, W. Lowther, K.A. Morano, J.D. West

BIOL 240. Conformational preferences in beta-sheet peptidomimetics. **B. Linton**

BIOL 241. Sirtuin 2 inhibitors identified by phage display with an expanded genetic code. **J.M. Tharp**, C. Reed, Y. Kurra, W. Liu

BIOL 242. Prolyl oligopeptidase family protein 2 (POP2): A protease with a taste for antibodies. **L. Jam**, C.M. Evilia

BIOL 243. Effect of the antimicrobial peptide combi-2 on lipid bilayers mimicking bacterial membranes. **B.M. Almarwani**, N. Phambu

BIOL 244. Demonstration of horizontal gene transfer from genetically engineered cyanobacteria to wild-type *E. coli*. **T. Nguyen**, **C. Barnes**, J. Agola, S. Sherazi, **L.H. Greene**, **J.W. Lee**

BIOL 245. Human glutathione synthetase: Negative cooperativity and substrate binding studies. A. Stopper, L. Haynes, I. Chavarri, H. Conrad Webb, **M.E. Anderson**

BIOL 246. LC-MS/MS-based analytical method for Marfey's reagent derivatized amino acid stereoisomers and it's application to biological samples. N.J. Ayon, **W.G. Gutheil**

BIOL 247. Trehalose monomycolate analogue containing a cleavable biotin affinity tag for labeling and identifying o-mycoloylated proteins in *Corynebacterineae*. **N. Banahene**, B.M. Swarts

BIOL 248. Analysis of *eyes shut* (EYS) function during intestinal regeneration in *Drosophila melanogaster*. **H. Cummins**, C. Penalva, J. Maldera, R. Sudhakaran, B.A. Edgar

BIOL 249. Series of cisplatin prodrugs to inhibit fatty acid oxidation in prostate cancer. **A.A. Kalathil**, S. Dhar

BIOL 250. Expanding the scope of RNA-TAG: From cell imaging to the conjugation of modified mRNA. **E.C. Zhou**, N.K. Devaraj

BIOL 251. Amyloid aggregation of the C-terminal peptide of BAX: A pro-apoptotic human protein. **D.A. Price**, K. Hutson, T.D. Hill, S.D. Moran

BIOL 252. Withdrawn

BIOL 253. Wireless handheld sensor for salivary cortisol detection. **A. Jangam**, N. Dave, P. Akhade, P. Manickam, **R.E. Fernandez**, S. Bhansali

BIOL 254. AdCasT: A single vector system for tunable control of genome-wide genetic perturbations. **C.L. Moore**, M. Shoulders

BIOL 255. Investigations into the development of new penetrating chaperones: Smuggling therapeutics across gram-negative bacteria and the blood-brain barrier. **R. Rafferty**, T. Nguyen, V. Hoang, P. Desman, A. Fatino

BIOL 256. Unveiling molecular mechanisms of kinesin-5 function using multiscale computational techniques. **A. Davtyan**, A. Kolomeisky, Q. Wang

BIOL 257. Connecting genes to molecules: Identifying novel small molecules in microbe-plant interactions. **E.M. O'Neill**

BIOL 258. Applications of multidimensional time model for PDF applied to Fokker- Planck equation and multi-scale time analysis to the rate of transcription or translation controlled by riboswitches. **M. Fundator**

BIOL 259. Ultraviolet light induced self-quenching of protein fluorescence. **M. Marlow**

BIOL 260. Withdrawn

BIOL 261. Identification of vaginal bacterial species that are mutually and differentially antagonistic with strains of Candida albicans. **A. Prenkocevic**

BIOL 262. Using dye molecules to study xenobiotic transport in the mosquito, *A. aegypti*. R. Arens, **M. Rouhier**

BIOL 263. Toward deciphering the biochemistry of DNA thymidine hypermodification in bacteriophages. **Y. Lee**, N. Dai, C. Guan, I. Correa, P.R. Weigele

BIOL 264. Characterization of the binding partners of MitoNEET. **M. Konkle**, K. Meenagh, R. Skolik, R. Guan, M. Menze, W.J. Geldenhuys

BIOL 265. Crustin and related putative antimicrobial peptides in the lobster, *Homarus americanus*: Identification using transcriptomics with top-down and bottom-up peptidomic strategies. **D. Do**, G.H. Vu, P.S. Dickinson, A.E. Christie, E.A. Stemmler

BIOL 266. Use of synthetic peptidomimetics for a critical evaluation of Aβ structure and functions. **S. Kumar**, A. Henning-Knechtel, M. Magzoub, A.D. Hamilton

BIOL 267. Oxidative damage affected by packaging density in sperm protamine-DNA complexes. **L.E. Prevette**, E. Merino, J.E. Derouchey

BIOL 268. High resolution measurement of membrane protein endocytosis. **Z. Zhang**, D.K. Heidary, C.I. Richards

BIOL 269. Molecular dynamics simulations of inhibition and disease mechanisms of metabolite fibrils. **P. Rehak**, P. Kral

BIOL 270. Dynamics of a π-stacked substrate analog in a flavoenzyme active site using 2D IR spectroscopy. **T.D. Hill**, H. Lepird, J. Zhu, D.A. Price, S.D. Moran

BIOL 271. Biosynthesis of the antimycobacterial lasso peptide, lariatin A, in *Escherichia coli*. **A. Adeniji-Adele**, M. Donohue, C. van Horn, J.W. Tomsho

BIOL 272. Allosteric activation by membranes regulates substrate specificity of lipolytic enzymes. **V. Mouchlis**, J. McCammon, E.A. Dennis

BIOL 273. Synthesis, spectroscopic investigation, biological screening, interaction with SS-DNA and DFT study of ferrocene-modified ureas. **F. Asghar**, A. Badshah, I.S. Butler

BIOL 274. Heterochiral DNA strand displacement circuits. **A. Kabza**, B. Young, J. Sczepanski

BIOL 275. Investigating the dienophile effect on the fluorogenic efficiency of cycloaddition reactions with tetrazines. **B. Pinto-Pacheco**, D. Buccella, S.A. Khan, W. Carbery, D. Turner

BIOL 276. Quantifying tetracycline resistance genes in swine waste anaerobic digester over a period of 100 days. **M. Couch**, G. Agga, J.H. Loughrin, R. Parekh, S. Antle, J. Kasumba, B. Couch, E.D. Conte

BIOL 277. Synthesis and evaluation of Nebraska Red derivatives for protein labeling studies. **L. Lesiak**, X. Zhou, C.I. Stains

BIOL 278. Noncovalent exocyclic methylene intermediate in flavin-dependent thymidylate synthase: Fact or artifact? **D. Mondal**, J. Yao, D. Quinn, A. Kohen

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 243

Mid-Career Investigators in Biological Chemistry

P.C. Bevilacqua, S.O. Kelley, *Organizers*
A. Miller, *Presiding*

8:00 Introductory Remarks.

8:05 BIOL 279. Small molecule-mediated delivery to human Langerhans cells. J. Schulze, E. Wamhoff, L. Bellmann, M. Rentzsch, R. Wawrzinek, G. Bachem, O. Seitz, P. Stoitzner, **C. Rademacher**

8:25 BIOL 280. Discovery of a covalent inhibitor of ERK docking-interactions that inhibits A375 melanoma tumor growth. **K.N. Dalby**

8:45 BIOL 281. Photoactive rhenium dipyridophenazine carbonyl complexes as sensors for protein aggregation and photochemical footprinting. A. Aliyan, T.J. Paul, C. Pennington, B. Jiang, G. Sharma, R. Prabhakar, **A.A. Marti**

9:05 BIOL 282. Impact of medium components on phospholipase B-like 2 protein levels in cell cultures. **Q. He**, J. Tian, Y. Qian, T. Straub, M. Rdultowki, B. Eagan, N. Vaidyanathan, C.L. Oliveira, E. Vandermark, C. Kramer, N. Qian, M.C. Borys

9:25 BIOL 283. Lipid transfer mechanism of cholesteryl ester transfer protein between HDL and LDL. **S. Senapati**

9:45 Intermission.

10:00 BIOL 284. Unleashing bacterial biosynthetic pathways to expand diketopiperazine chemical diversity. **A. Lane**, R. Viswanathan, R. Lopez, J. Carey, P. Borgman, E. James, C. Webb

10:20 BIOL 285. High-efficiency "-1" and "-2" ribosomal frameshiftings revealed by force spectroscopy. **Y. Wang**

10:40 BIOL 286. Role of cathepsin L in β-synuclein degradation. R.P. McGlinchey, S.M. Lacy, **J.C. Lee**

11:00 BIOL 287. 1β-2-Himachalen-6-ol: A novel anticancer sesquiterpene unique to the Lebanese wild carrot. **R.I. Taleb**, C. Daher, M. El Sibai, M. Mroueh

11:20 BIOL 288. Small oxoacids of sulfur (SOS) and selenium (SOSe). **P.J. Farmer**, M. Kumar

11:40 BIOL 289. Energy-conserving bifurcating activity in electron-transfer flavoproteins. H.D. Duan, N.M. Raseek, G.J. Schut, D. Nguyen, M.W. Adams, **A. Miller**

Section B
Ernest N. Morial Convention Center
Room 244

Graduate Student & Postdoctoral Fellow Symposium

P.C. Bevilacqua, S.O. Kelley, *Organizers*
C. Berman, *Presiding*

8:30 Introductory Remarks.

8:35 BIOL 290. Molecular evolution of densely-functionalized aptamers. **D. Kong**, W. Yeung

8:50 BIOL 291. Toward RNA life: Synthesis and replication of RNA by RNA. **D.P. Horning**, S. Bala, J.C. Chaput, G.F. Joyce

9:05 BIOL 292. Capping 5′-triphosphate oligonucleotides with vaccinia virus capping enzyme. **M. Wulf**, P. Humbert, J.L. Buswell, I. Schildkraut, I. Correa

9:20 BIOL 293. Using computationally-engineered promiscuous EF-Tu variants to more efficiently translate unnatural amino acids. **V. Cox**, E.A. Gaucher

9:35 BIOL 294. Enzymatic site-specific labeling of RNA for affinity isolation of RNA-protein complexes. **K.N. Busby**, N.K. Devaraj

9:50 BIOL 295. Construction of designer chromatin with unique multi-functional DNA sequence: Effect of chromatin topology in base excision repair. **D. Banerjee**, C. Deckard, J. Sczepanski

10:05 Intermission.

‡*Cooperative Cosponsorship*

10:20 BIOL 296. Using protected triazabutadienes for aryl diazonium ion generation. **L. Guzman**

10:35 BIOL 297. Chemical tools for protein imaging in live bacterial cells. **S.H. Ho**, D.A. Tirrell

10:50 BIOL 298. Compatible bioorthogonal reactions for multicomponent labeling. **S. Nguyen**, D. Row, D.N. Kamber, J.A. Prescher

11:05 BIOL 299. Engineering post-translational proofreading to discriminate non-standard amino acids. A.M. Kunjapur, **D. Stork**, E. Kuru, O. Vargas-Rodriguez, M. Landon, D. Söll, G.M. Church

11:20 BIOL 300. Continuous directed evolution in human cells. **C. Berman**, L.J. Papa, S.J. Hendel, C. Moore, P. Suen, A. Weickhardt, M. Shoulders

11:35 BIOL 301. Targeting mutations to specific genes in living systems. **L.J. Papa**, C.L. Moore, M. Shoulders

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 243

Protein Homestasis

S.O. Kelley, *Organizer*
M. Shoulders, *Organizer, Presiding*

1:30 BIOL 302. Host proteostasis modulates RNA virus evolution. **M. Shoulders**

2:05 BIOL 303. Sil1, the ER Hsp70 co-chaperone, plays a critical role in maintaining skeletal muscle proteostasis and physiology. **L. Hendershot**

2:40 BIOL 304. The chaperome in cancer – a chemical biology approach. **G. Chiosis**

3:15 Intermission.

3:35 BIOL 305. A HaloTag-based multi-color fluorogenic sensor to visualize and quantify proteome stress in live cells. Y. Liu, M. Fares, **X. Zhang**

4:10 BIOL 306. Methods to enable regulated gene therapy. **T.J. Wandless**

Section B
Ernest N. Morial Convention Center
Room 244

Graduate Student & Postdoctoral Fellow Symposium

P.C. Bevilacqua, *Organizer*
S.O. Kelley, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 BIOL 307. Genetically targeted tetramethylrhodamine voltage reporters. **P. Deal**, P. Liu, S. Al-Abdullatif, E. Miller

1:50 BIOL 308. Expanding the bioluminescent toolbox with pi-extended luciferins. **Z. Yao**, B.S. Zhang, J.H. Mills, J.A. Prescher

2:05 BIOL 309. Targeted drug delivery in 2- and 3D cultured cells by two-photon activation of a nitrodibenzofuran-caged farnesyltransferase inhibitor. **M. Hammers**, M.D. Distefano

2:20 BIOL 310. Targeting cancer stem cells with molecular imaging probes. **T. Bearrood**, C. Anorma, N. Pino, S. Dibrell, J. Chan

2:35 BIOL 311. Withdrawn

2:50 BIOL 312. Development of novel far-red to near-infrared fluorophores for chemical biology. **X. Zhou**, L. Lesiak, Y. Fang, R. Lai, C. Elowsky, H. Li, C.I. Stains

3:05 Intermission.

3:20 BIOL 313. Tunable polymeric lysosomal rupture probe to investigate mechanism of NLRP3 Inflammasome activation. **S. Manna**, W.J. Howitz, N.J. Oldenhuis, A. Eldredge, M. Lodeon, Z. Guan, A.P. Esser-Kahn

3:35 BIOL 314. Post-translational thioamidation of methyl-coenzyme M reductase, a key enzyme in the global carbon cycle. **N. Mahanta**, D. Nayak, A. Liu, S. Dong, S. Nair, W. Metcalf, D. Mitchell

3:50 BIOL 315. The Trpm7 kinase domain regulates breast cancer cell migration and tumor metastasis. **T.S. Kaoud**, X. Xie, R.A. Mangieri, J. Park, C.D. Tavares, N.D. Ebelt, S. Van Ravenstein, M. Cano, S. Mitra, M.F. Radwan, R.A. Morrisett, C. Bartholomeusz, K.N. Dalby

4:05 BIOL 316. Development of a bioreducible *N*-oxide-based probe for photoacoustic imaging of hypoxia. **H.J. Knox**, J. Hedhli, T. Kim, K. Khalili, L. Dobrucki, J. Chan

4:20 BIOL 317. Carbofluorescein voltage indicators for studying membrane potential. **G. Ortiz**, P. Deal, P. Liu, S. Naing, E. Miller

4:35 BIOL 318. Using glycosaminoglycan mimetics to influence stem cell differentiation. **M. Naticchia**, L. Laubach, K. Godula

WEDNESDAY EVENING

Biomineralization & Bio-Compatible Minerals
Sponsored by GEOC, Cosponsored by BIOL and ENVR

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

BMGT

Division of Business Development & Management

J. Cohen and A. DeMasi, *Program Chairs*

SUNDAY MORNING

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

SUNDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon B Sec 7

Chemical Angel Network (CAN): Chemists Investing in Chemistry-Based Companies
Cosponsored by PROF and SCHB‡
Financially supported by CIEC
J.L. Bryant, M. Vreeke, *Organizers*
S.S. White, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 BMGT 1. Updates and news from the Chemical Angel Network (CAN) and its fifth year of supporting chemists and chemistry-based company creation. **M. Vreeke**, S.S. White, J.C. Giordan

2:00 Company Presentations.
3:00 Investment Discussion.
3:30 Open Forum.
4:00 Concluding Remarks.

MONDAY MORNING

Issues in Chemical Commercialization
Sponsored by CHAL, Cosponsored by BMGT

MONDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon B Sec 7

Thriving in the Workplace: Non-Technical Skills that Boost your Value
Cosponsored by PROF‡, SCHB, WCC‡ and YCC‡
L. Dulany, *Organizer, Presiding*

2:00 Introductory Remarks.

2:10 BMGT 2. Soft skills in hiring in the government sector and the link to diversity. **D. Strong**

2:35 BMGT 3. Thriving in the workplace: Collaboration is the key to success. **J.M. Iriarte-Gross**

3:00 BMGT 4. Emotional intelligence and the repertoire of non-technical skills. **L.S. Sremaniak**

3:25 BMGT 5. How you are who you are makes all the difference. **L. Dulany**

3:50 BMGT 6. Caring for your brand and your career. **W.F. Carroll**

4:15 Concluding Remarks.

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix

J.L. Bryant, A.S. DeMasi, *Organizers*

8:00–10:00

BMGT 7. Procurement strategies for managing technologies. **R.F. Burgoyne**

BMGT 8. Entrepreneurship and innovation for scientists in Puerto Rico. **A.G. Colon Santiago**, U.M. Cordova-Figueroa, **J.I. Ramirez Domenech**, E. Ferrer Torres, O.J. Morales Martinez, M. De Hoyos, M. Otaño

CARB

Division of Carbohydrate Chemistry

S. Sucheck, *Program Chair*

SUNDAY MORNING

Section A
Loews New Orleans Hotel
Feliciana West

Wolfrom Award

E. Rozners, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 CARB 1. Chemical probes of glycan assembly in microbes. **L.L. Kiessling**

10:10 Discussion.

10:15 CARB 2. Human milk oligosaccharides in antimicrobial chemotherapy. **S.D. Townsend**

10:50 Discussion.

10:55 CARB 3. Building oligosaccharides and building community. **N.L. Pohl**

11:30 Discussion.

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

SUNDAY AFTERNOON

Section A
Loews New Orleans Hotel
Feliciana West

Isbell Award

E. Rozners, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CARB 4. Carbohydrate chemistry in the service of anti-infective drug discovery. **D. Crich**

2:00 Discussion.

2:05 CARB 5. Synthesis as an enabling technology for understanding bacterial glycan biosynthesis and function. **T.L. Lowary**

2:30 Discussion.

2:35 CARB 6. Approaches to 1,2-*cis*-2-aminosugars and heparan sulfate mimicking glycopolymers . **H.M. Nguyen**

3:00 Discussion.

Section A
Loews New Orleans Hotel
Feliciana West

Gin New Investigator Award

E. Rozners, *Organizer, Presiding*

3:25 Introductory Remarks.

3:30 CARB 7. Expedient methods for the stereocontrolled synthesis of oligosaccharides. **C. Bennett**

3:55 Discussion.

4:00 CARB 8. Allostery in C-type lectins. J. Hanske, S. Aleksić, J. Aretz, H. Baukmann, R. Wawrzinek, J. Schulze, B. Keller, **C. Rademacher**

4:25 Discussion.

‡*Cooperative Cosponsorship*

4:30 CARB 9. Genetically-encoded toolbox for discovery of ligands for glycan-binding proteins (GBPs). **R. Derda**

4:55 Discussion.

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

MONDAY MORNING

Section A
Loews New Orleans Hotel
Feliciana West

Horton Award

E. Rozners, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 CARB 10. Building drug delivery systems: *In vitro* and *in vivo* studies of drug-hydroxybutenyl cyclodextrins complexes. **C.M. Buchanan**

10:10 Discussion.

10:15 CARB 11. Cyclodextrins in the therapy of Niemann-Pick C disease. **K. Dobrenis**, C. Davidson, A. Smith, S. Walkley

10:50 Discussion.

10:55 CARB 12. Cyclodextrins from toy to tool: Excipients and therapeutic agents. **L. Szente**

11:30 Discussion.

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

MONDAY AFTERNOON

Section A
Loews New Orleans Hotel
Feliciana West

Advances in Molecular Recognition of Double-Helical DNA & RNA
Cosponsored by MEDI and ORGN
Financially supported by Shimadzu, Glen Research
E. Rozners, *Organizer*
D.P. Arya, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CARB 13. Sequence-based design of potent and selective small molecules targeting RNA. **M.D. Disney**, H. Haniff, M. Costales, A. Angelbello, S. Velagapudi, S. Rzuczek

2:05 CARB 14. Design and synthesis of pi-extended nucleobases for sequence selective triple-helical recognition of RNA using peptide nucleic acids . **J.A. MacKay**, A.K. Williams, H.A. Sofka, E. Rozners

2:35 CARB 15. Narrowing the gap between affinity and efficacy with RNA-targeted peptidomimetics. **B.L. Miller**, V. Anokhina, J.D. McAnany, O. Swart, T. Hilimire, J. Chamberlain, S. Dewhurst

3:05 Intermission.

3:25 CARB 16. Sequence-targeted invasion of DNA and RNA G quadruplexes by peptide nucleic acid. **B.A. Armitage**

3:55 CARB 17. Structural plasticity in disease and pharmaceutical targeting of non-coding RNAs. **G. Varani**

4:25 Concluding Remarks.

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Sponsored by CELL, Cosponsored by AGFD, ANYL and CARB

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix

S.J. Sucheck, *Organizer*

8:00–10:00

35, 37-38, 41-44, 46-48, 50, 54-55, 57, 62, 65, 70-71, 79. See subsequent listings.

TUESDAY MORNING

Section A
Loews New Orleans Hotel
Feliciana West

Recent Advances in Catalytic Carbohydrate Reaction Development
Cosponsored by ORGN
W. Tang, *Organizer*
H.M. Nguyen, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CARB 18. NIH glycoscience program: Developing new facile methods for synthesis of biomedically relevant carbohydrates. **P. Marino**

8:50 CARB 19. Cell-surface glyco-engineering using sialyl transferases and modified CMP-Neu5Ac derivatives. **G. Boons**

9:20 CARB 20. Chemoselective amidoglycosylation of all four D-glycal 3-carbamate diastereomers: Synthesis of stereo-varied 2-amino sugar oxazolidinones. **C.M. Rojas**

9:50 Intermission.

10:10 CARB 21. Challenges in automating catalytic glycosylation methods. **N.L. Pohl**

10:40 CARB 22. One-pot multienzyme (OPME) chemoenzymatic synthesis of carbohydrates and sialidase inhibitors. **X. Chen**

11:10 CARB 23. Regenerative glycosylation via nucleophilic catalysis. **A. Demchenko**, Y. Singh, K.J. Stine

Section B
Loews New Orleans Hotel
Louisiana II

Advances in Molecular Recognition of Double-Helical DNA & RNA
Cosponsored by MEDI and ORGN
Financially supported by Shimadzu, Glen Research
D.P. Arya, *Organizer*
E. Rozners, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 CARB 24. Optical control of nucleic acid function in biological systems. **A. Deiters**

9:35 CARB 25. Molecular recognition of DNA: From discovery to oncology. **A. Kurmis**, P.B. Dervan

10:05 CARB 26. Modulating nucleic acid structure and function using shape-selective small molecules. **D.M. Chenoweth**

10:35 Intermission.

10:55 CARB 27. Small molecule therapeutics targeting nucleic acids. **D.P. Arya**

11:25 CARB 28. Target-specific inhibition of transcription factors by designed, synthetic DNA ligands. **W. Wilson**, A. Paul, P. Guo, T.D. Vo, N. Harika, A. Kumar, A.A. Farahat, B. Liu, G.M. Poon, M.W. Germann, B.W. David

11:55 Concluding Remarks.

TUESDAY AFTERNOON

Section A
Loews New Orleans Hotel
Feliciana West

Recent Advances in Catalytic Carbohydrate Reaction Development
Cosponsored by ORGN
H.M. Nguyen, *Organizer*
W. Tang, *Organizer, Presiding*

1:30 CARB 29. De novo approaches to oligosaccharide assembly for stereochemical structure activity relationship studies (S-SAR). **G.A. O'Doherty**

2:00 CARB 30. Silane reagents for intramolecular glycosylation. **J. Montgomery**

2:30 CARB 31. Pd-catalyzed asymmetric hydroalkoxylation of allene: A new synthetic method for carbohydrates. **Y. Rhee**, M. Kim, J. Lee, S. Kang

3:00 Intermission.

3:20 CARB 32. Production of O-glycans and O-glycopeptides/glycoproteins by chemical and enzymatic catalysis production of *O*-glycans and *O*-glycopeptides/glycoproteins by chemical and enzymatic catalysis. **P.G. Wang**

3:50 CARB 33. New catalytic methods in carbohydrate synthesis. **M.A. Walczak**

4:20 CARB 34. New catalytic methods for stereoselective glycosylation. **H.M. Nguyen**

Discovery of Small Molecules Targeting RNA
Sponsored by ORGN, Cosponsored by CARB and MEDI

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

General Posters

S.J. Sucheck, *Organizer*

7:30–9:30

CARB 36. New metabolic chemical reporter 6-azido-6-deoxy-glucose reveals an unexpected substrate promiscuity of O-GlcNAc transferase and the potential for protein modification by O-glucose. **N. Darabedian**, M. Pratt

CARB 35. Synthesis and biological evaluations of mono- and poly-fluorogalactopyranosides: Preparation of selective galectin inhibitors. **D. Laine**, V. Denavit, D. Giguere

CARB 37. Direct coupling of amides and urea to glycosyl halides using silver triflate. **M. De Castro**

CARB 38. Improved HPAE-PAD method for glycoprotein monosaccharide determination. **S. Patil**, J. Rohrer

CARB 39. Synthesis of the glycosylated amino acid bearing the Thomsen nouvelle antigen. **E.R. Mercer**, D. Beckwith, M. Cudic

CARB 40. Comparison of furanoside conformational preferences between calculation and better resolved NMR measurement. **J.S. Rhoad**, S. Culver

CARB 41. Withdrawn

CARB 42. Isoquinoline-1-carboxylate as a traceless leaving group for chelation-assisted glycosylations. **C. Simmons**, H. Wang, W. Tang

CARB 43. Electrostatic control of binding interactions etween ETS transcription factors proteins and theirs cognate DNA. **T.D. Vo**, S. Wang, G.M. Poon, W. Wilson

CARB 44. Using chiral catalysts and cation-*n* interactions to direct site-selective acylation of carbohydrates. G. Xiao, **S. Blaszczyk**, G. Cintron-Rosado, D.A. Glazier, P. Liu, W. Tang

CARB 45. Divergent stereoselective synthesis of rare amino-sugars. **D.A. Glazier**, Z. Zhu, W. Tang

CARB 46. Development of a new class of carbohydrate-based adjuvants. **C.E. Marzabadi**, V. Basava, C. Bitsaktsis, D. Nichols

CARB 47. A selective small-molecule inhibitor of O-GlcNAc transferase. **N. Pedowitz**

CARB 48. Glycosidase inhibition by multivalent presentation of heparan sulfate saccharides on bottlebrush polymers. **E. Sletten**, R. Loka, H.M. Nguyen

CARB 49. Application of indium bromide catalyst to the synthesis of disaccharides. **G.W. Lang**

CARB 50. Minimalist approach to assemble complex saccharides with unprotected donors. **G. Bati**, K. Le Mai Hoang, J. He, M. Chan-Park, X. Liu

CARB 51. Analysis of glycoprotein production in antibiotic resistant strains of *Helicobacter pylori*. **H. Blain**, D.H. Dube

CARB 52. Targeting of *Helicobacter pylori* using photodynamic therapy agents. **D. Williams**, **D.H. Dube**

CARB 53. Withdrawn

CARB 54. Using density variant microarrays to investigate the effect of glycan presentation on viral binding. **T. Lucas**, C.J. Fisher, K. Godula

CARB 55. Withdrawn

CARB 56. Chemical reporter for dual cell-surface labeling of mycobacteria.

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D.J. Moore, H.W. Kavunja, T. Nathan, B.M. Swarts

CARB 57. Structural and functional analysis of the *N*-acetylglucosamine-6-phosphate deacetylase (NagA) from *Mycobacterium tuberculosis*. **E. Fullam**

CARB 58. Synthesis and evaluation of cell-permeable trehalose analogues for the protection of mammalian cells . **T.E. Williamson**, M.G. Paulick

CARB 59. A kinetic study of porcine liver esterase hydrolysis of cell-permeable analogues of trehalose . **G.A. Hayner**, A.M. Bannister, M.G. Paulick

CARB 60. Withdrawn

CARB 61. Synthesis and evaluation of butyrylated trehalose analogues for the protection of mammalian cells. **R.A. Riley**, M.G. Paulick

CARB 62. Synthesis of fluorescence resonance energy transfer (FRET)-based fluorogenic probes for the investigation of arabinogalactan mycolate metabolism in mycobacteria. **D. Wing**, B.M. Swarts

CARB 63. Possible aggregation effect in fluorous-tagged oligosaccharide synthesis. **A.G. Gonzalez**, I.H. Mahmud, Z. Shahin, P. Goekjian

CARB 64. Concise chemoenzymatic synthesis of trehalosamine, an aminoglycoside antibiotic and precursor to mycobacterial imaging probes. **J.M. Groenevelt**, L.M. Meints, A.I. Stothard, A. Poston, P. Woodruff, B.M. Swarts

CARB 65. Chemoenzymatic desymmetrization of a potential synthetic precursor of bioactive *myo*-inositol phosphates. **A.B. Simas**, B.S. de Jesus, M.F. Ribeiro, D.M. Freire, E.A. Manoel

CARB 66. Chemoenzymatic synthesis and evaluation of 5-deoxy-thio-D-trehalose as a trehalase-resistant trehalose surrogate. **N.D. Danielson**, B.M. Swarts

CARB 67. Heterobifunctionalized poly(ethylene glycol) and poly(propylene glycol) polymers for bioconjugation applications. **J. Blankenship**, K. Yoshimatsu

CARB 68. Glycan engineering for 3D embryonic stem cell bodies. **L. Laubach**, M. Naticchia

CARB 69. Exploring the chemistry and the bonding in oligosaccharides derived from sugars and sugar acids . **M. Schmid**, C.L. Liotta

CARB 70. Effect of silyl groups at C-4 in sialyation reactions. **M. Lohman**, C. De Meo

CARB 71. Effects of side chain conformation in chemical sialylations of Neu5Ac derivatives via 8,9-O-substitution . **B. Jones**, C. De Meo

CARB 72. Selective acetylation on sialic acid donors. **S. Ritter**, M. Shadrick, C. De Meo

CARB 73. A non-woven fabric wound dressing containing layer-by-layer deposited hyaluronic acid and chitosan. **A. Ahmed**, H. Fahmy, A. Ahmed Ali

CARB 74. Withdrawn

CARB 75. Investigation of accelerated hydrolysis of cellulose after chemical modification. **B. Mu**, H. Xu, Y. Yang

CARB 76. One-pot gram-scale synthesis of GlcNAcylated amino acids via indium bromide catalysis. **C.A. Deleon**, M. Pratt

CARB 77. Efficient catalytic conversion sugar-rich microalgae into glycol, lactic acid and HMF in water. **L. Kong**, Z. Tan, G. Miao, Y. Sun

CARB 78. Mechanistic studies on the catalytic transformation of glucose over acid or base catalysts. L. Shi, **S. Li**, L. Kong

CARB 79. BF_3–*N*,*N*–dimethylformamide catalyst for synthesis minimally protected 1,2-*cis*- glycopyranosides in solution and solid-phase stereocontrolled synthesis. **G. St-Pierre**, S. Hanessian

WEDNESDAY MORNING

Section A
Loews New Orleans Hotel
Feliciana West

Emerging Young Investigator Symposium

K. Godula, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 CARB 80. Trying to identify and address grand challenges in carbohydrate science. **B.G. Davis**

9:40 CARB 81. Chemical tools and strategies to decipher the role of glycans in human disease. **M.A. Walczak**

10:05 CARB 82. Mono- and poly-fluorinated carbohydrates: Synthetic challenges associated to a new class of bioactive molecules. **D. Giguere**, V. Denavit, D. Lainé

10:30 Intermission.

10:45 CARB 83. Substrate recognition of reversible O-GlcNAcylation. **J. Jiang**

11:10 CARB 84. Exploiting the inhibitory function of CD22 on B-cells to prevent antibody responses. **M.S. Macauley**, B. Arlian, K.J. Bednar, S. Duan, W. Fung-Leung, M.D. Kulis, L. Hardy, C. Nycholat, K.A. Orgel, L. Pang, J.C. Paulson, T.S. Rao

11:35 CARB 85. Commandeering mycobacterial carbohydrate metabolism for applications in tuberculosis research. **B.M. Swarts**

Section B
Loews New Orleans Hotel
Pointe Coupee

Recent Advances in Catalytic Carbohydrate Reaction Development
Cosponsored by ORGN
W. Tang, *Organizer*
H.M. Nguyen, *Organizer, Presiding*

9:00 CARB 86. Towards catalytic site-selective alterations of glycopeptide antibiotics and other carbohydrates . **S.J. Miller**

9:30 CARB 87. Coinage metal-catalyzed stereoselective glycosidic bond formation. **L. Zhang**

10:00 CARB 88. Studies on regioselective glycosylation of natural polyols. **P. Nagorny**, J. Tay, A.J. Arguelles, M. DeMars III, P.M. Zimmerman, D.H. Sherman

10:30 Intermission.

10:50 CARB 89. Organoboron catalysts and reagents for carbohydrate chemistry. **M.S. Taylor**

11:20 CARB 90. Chiral catalyst-directed site-selective functionalization of carbohydrates . **W. Tang**

11:50 Concluding Remarks.

Plant Heteropolysaccharides: Interactions within Lignocellulosics, New Modifications & Future Applications

Structures, Interactions, & Extraction of Plant Heteropolysaccharides

Sponsored by CELL, Cosponsored by CARB

Discovery of Small Molecules Targeting RNA: Where Are We & Where Are We Going?
Sponsored by MEDI, Cosponsored by CARB and ORGN

WEDNESDAY AFTERNOON

Section A
Loews New Orleans Hotel
Feliciana West

Emerging Young Investigator Symposium

K. Godula, *Organizer, Presiding*

2:00 CARB 91. Anti-pathogenic glycoconjugates. **S.D. Townsend**

2:25 CARB 92. Solving puzzles of glycoside hydrolase reaction mechanisms. **H. Mayes**

2:50 CARB 93. Mimetic sugar-nucleotides to probe a strategic bacterial dehydrogenase enzyme. **G.J. Miller**, S. Ahmadipour, L. Beswick

3:15 Intermission.

3:30 CARB 94. Synthetic glycoproteins by polymerization of glycosylated NCAs . **J. Kramer**

3:55 CARB 95. Self-assembling glycopeptide hydrogels as selectively permeable mucus-like barriers. **G. Hudalla**, A. Restuccia

4:20 Concluding Remarks.

Plant Heteropolysaccharides: Interactions within Lignocellulosics, New Modifications & Future Applications

Modification & Future Applications of Plant Heteropolysaccharides

Sponsored by CELL, Cosponsored by CARB

CATL

Division of Catalysis Science and Technology

A. Savara, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent (see COLL, Sun, Mon, Tue)

Surface Chemistry (see *COLL*, Sun, Mon, Wed, Thu)

Natural Gas Catalysis (see *ENFL*, Sun)

Roadmap & Policy of Energy & Fuels (see *ENFL*, Mon, Tue, Wed)

Metal-Organic Frameworks: What Are Next? (see *INOR*, Sun, Mon, Tue, Wed)

SOCIAL EVENTS:

CATL Social Hour, 6:30 PM: Mon

BUSINESS MEETINGS:

CATL Executive Board Meeting, 5:30 PM: Mon

SUNDAY MORNING

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms & Selectivity

Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

8:00 CATL 1. Reactions of oxygenates on well-defined Lewis acid sites in zeolite BEA. **C. Sievers**, J. So, D. Sholl

8:20 CATL 2. The mechanism and kinetics of acetone condensation to methyl isobutyl ketone. **A.T. Bell**

9:00 CATL 3. Controlling the selectivity in CO_2 reduction over Pd/Al_2O_3 catalysts through mechanistic understanding: A SSITKA/*operando* FTIR study. **J. Szanyi**, X. Wang, H. Shi, N. Nelson

9:40 Intermission.

10:00 CATL 4. Understanding mechanocatalytic reaction pathways: Surface chemistry at the solid-solid interface. **W.T. Tysoe**

10:40 CATL 5. Nature of active sites and surface intermediates during SCR of NO with NH_3 by supported V_2O_5-WO_3/TiO_2 catalysts. M. Zhu, J. Lai, U. Tumuluri, Z. Wu, **I.E. Wachs**

11:20 CATL 6. Interrogating supported oxides in confined environments using site titration techniques. A. Ardagh, D. Bregante, D. Flaherty, **J.M. Notestein**

11:40 CATL 7. Synthesis-property-mechanism relationships for catalysts via statistically guided methods. **J. Lauterbach**

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Section B
Hampton Inn & Suites Convention Center
Riverside I

Control of Zeolite Structure, Composition & Sites for Catalysis
Cosponsored by INOR
S. Goel, R. Gounder, W.F. Schneider, *Organizers, Presiding*

8:00 CATL 8. Unraveling active site identity in Lewis acid zeolites using MAS NMR of adsorbed probe molecules. **Y. Roman-Leshkov**

8:20 CATL 9. Cooperative effects of structure-directing agents in zeolite synthesis. **J.D. Rimer**, R. Li, M. Kumar, W. Qin, A. Chawla

9:00 CATL 10. Impact of starting materials on the Al distribution of the CHA-type aluminosilicate zeolites. **T. Yokoi**, T. Nishitoba

9:20 CATL 11. Ab initio quantum chemistry for understanding active sites in zeolites. **J. Sauer**

10:00 Intermission.

10:15 CATL 12. Ex-situ and in situ liquid imaging of zeolites in the scanning transmission electron microscope. **I. Arslan**

10:35 CATL 13. Computational prediction of chemically-synthesizable organic structure directing agents for zeolites. **M.W. Deem**

11:15 CATL 14. Noble metals in small-pore zeolites. **P. Serna Merino**, J. Gabay, R. Carr, C. Kliewer, G. Casty, J. Guzman, M. Moliner, A. Corma

11:35 CATL 15. On the influence of catalyst acid strength in the methanol to hydrocarbons (MTH) and related reactions. M. Mortén, L. Mentel, A. Lazzarini, I. Pankin, C. Lamberti, S. Bordiga, V. Crocella, S. Svelle, K. Lillerud, **U. Olsbye**

Section C
Hampton Inn & Suites Convention Center
Riverside III

Machine Learning for Catalysis Research
Cosponsored by CINF and COMP
J.R. Kitchin, A. Peterson, H. Xin, *Organizers, Presiding*

8:00 CATL 16. From process to properties: Correlating synthesis conditions, structural disorder and the catalytic performance of metallic nanoparticles. **B. Sun**, A.S. Barnard

8:20 CATL 17. Machine learning predictions of factors affecting the activity of heterogeneous metal catalysts. **I. Takigawa**, K. Shimizu, K. Tsuda, S. Takakusagi

8:40 CATL 18. Model based catalyst discovery from an industrial perspective. **E. Ras**

9:00 CATL 19. Choosing the right chemical representation for machine-learning-accelerated discovery and design in transition metal catalysis. **H.J. Kulik**

9:20 CATL 20. Application of machine learning tools for complex catalytic systems. **A. Heyden**

9:50 Intermission.

10:10 CATL 21. Combinatorial study of oxidation catalysts: Uncovering structure-activity relationships. **K. Mingle**, C. Wen, E. Sasmaz, J. Lauterbach

10:30 CATL 22. Addressing chemical complexity with surrogate models in computational catalyst design. **Z. Ulissi**

10:50 CATL 23. Machine (&human!) learning in catalyst discovery. Z. Li, S. Wang, **H. Xin**

11:10 CATL 24. Computationally-driven design of cation-based catalysts for ethene conversions. S.L. Pellizzeri, A. Samstag, I.A. Jones, H.A. Doan, V. Bernales, M. Barona, L. Gagliardi, R. Snurr, **R.B. Getman**

11:30 CATL 25. Accelerating discovery of catalysts and catalytic morphology. **T. Bligaard**

Section D
Hampton Inn & Suites Convention Center
Bienville

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Cosponsored by COMP, ENFL and PHYS
K. Schwarz, R. Sundararaman, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 26. Interfacing electrochemistry. **N. Markovic**

8:45 CATL 27. Hybrid methodology of modeling of the electrochemical dissolution of gold in the presence of specifically adsorbing ions. **A. Baskin**, C. Valero-Vidal, Z. Liu, D. Prendergast, E. Crumlin

9:05 CATL 28. Ion dynamics at the electrode-electrolyte interface. **A. Willard**

9:45 Intermission.

10:00 CATL 29. Modeling electrochemical reactions: DFT-based models including explicit solvation, electrolyte, and electrochemical potential. **J. Goodpaster**

10:20 CATL 30. Towards efficient N_2 electroreduction to ammonia through DFT investigation on surface environment and surface termination. **Y. Li**, S. Maheshwari, G. Rostamikia, M.J. Janik

10:40 CATL 31. First principles simulations of interfaces between photoabsorbers, water and catalysts. **G.A. Galli**

11:20 CATL 32. Coarse-grained models of electrochemically driven, open systems: The importance of constant potential boundary conditions and interfacial fluctuations. **K. Dwelle**, A. Willard

Section E
Hampton Inn & Suites Convention Center
Fulton

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Cosponsored by ENFL, INOR and PHYS
C.A. Carrero, R.B. Getman, I. Hermans, *Organizers, Presiding*

8:00 CATL 33. Crucial role of metastable structures of Pt clusters for light alkane activation. **P. Sautet**, G. Sun

8:40 CATL 34. Propane dehydrogenation over supported iron catalysts. S. Tan, M.L. Sarazen, S. Nair, **C.W. Jones**

9:00 CATL 35. C-H activation chemistry at phosphide surfaces. **W.F. Schneider**, J. Ko

9:20 CATL 36. New fundamental molecular level insights into oxidative coupling of methane (OCM) by SiO_2-supported tungstate catalysts. M. Zhu, Z. Fink, W. Taifan, M.E. Ford, F. Tielens, J. Baltrusaitis, **I.E. Wachs**

9:45 Intermission.

10:00 CATL 37. Understanding and tuning catalytic materials For methane activation using nanocrystal precursors. **M. Cargnello**, J. Willis, E. Goodman, C. Wrasman, A. Yang, F. Abild-Pedersen

10:20 CATL 38. Realities of cluster catalysts: Critical role of fluxionality, structural diversity in the ensemble, and presence of metastable sites. **A. Alexandrova**

10:40 CATL 39. Transition metal post-modifcation of MOFs: Vapor-phase syntheses and catalytic screening. I. Kim, M. Ferrandon, M. Delferro, **A.B. Martinson**

11:00 CATL 40. Control of the surface reactivity towards carbon, oxygen, and hydrogen over intermetallic compounds. Y. He, Y. Song, **S. Laursen**

11:20 CATL 41. Doped nickel oxides prepared by solventless synthesis: Ethane oxidative dehydrogenation performance and characterization. H. Zhu, M. Harb, D. Anjum, M. Hedhili, S. Ould-Chikh, J.M. Basset, **D. Rosenfeld**

11:40 CATL 42. Activation of hydrocarbons in catalytic reactors. **B.J. Tatarchuk**

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Challenge & Opportunity in Lignin Valorization
Cosponsored by ENFL, ENVR, INOR and PHYS
G. Beckham, *Organizer*
M.M. Abu-Omar, F. Wang, *Organizers, Presiding*

8:00 CATL 43. Reductive conversion of lignin with metal-doped catalysts. **M.B. Foston**

8:20 CATL 44. HDO of guaiacol over Ag/TiO_2 catalyst. **K. Liu**, Z. Zhang, M. Janik, S. Bai, G. Hou

8:40 CATL 45. Catalytic valorisation of industrial 2G biomass stillage into monomeric phenolics using Ru catalyst supported on 1D multiwall carbon nanotubes (Ru-MWCNT) with enhanced molecular accessibility. B. Gómez-Monedero, M. Ruiz-Ramiro, F. Bimbela, **J. Faria**

9:00 CATL 46. Lignin first approach using a continious flow system. I. Kumaniaev, E. Subbotina, M.V. Galkin, **J.S. Samec**

9:20 Intermission.

9:30 CATL 47. Stabilization with aldehydes for the high yield and high selectivity production of lignin monomers during integrated biomass depolymerization. **J. Luterbacher**

9:50 CATL 48. Lignin valorisation: Towards high added value chemicals, materials and fuels. **R. Luque**

10:10 CATL 49. Strategies for catalytic biofeedstock related conversions. **T.J. Marks**

10:30 CATL 50. Complete conversion of lignocellulose with integrated catalyst recycling: sustainable pathways to valuable chemicals and fuels. **K. Barta**

10:50 CATL 51. *Operando* kinetic and mechanistic study of catalytic hydrogenolysis of lignin β-O-4 ether linkage with supported metals. **L. Qi**, A. Chamas, D.W. Hoyt, E.D. Walter, N. Washton, S.L. Scott

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Synthetic Chemistry Addressing Challenges in Energy & the Environment
Sponsored by INOR, Cosponsored by CATL and WCC

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

SUNDAY AFTERNOON

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms at the Atomic Scale

Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

1:00 CATL 52. Kinetics and mechanism of alcohol conversion over shape-controlled oxide nanocrystals. G. Foo, G. Hu, D. Jiang, **Z. Wu**

1:20 CATL 53. CO oxidation on supported Ir and Pt single atoms: Structural and kinetic study. Y. Lu, C. Kuo, X. Zhang, J. Wang, H. Xin, **A.M. Karim**

2:00 CATL 54. Theoretical investigation of the reactivity of oxo compounds on ceria. C. Zhao, **Y. Xu**

2:40 Intermission.

3:00 CATL 55. Modifying metal nanoparticle surfaces to influence hydrogen transfer and oxygen dissociation for the direct synthesis of H_2O_2. **D. Flaherty**, N.M. Wilson, P. Priyadarshini, J. Adams

‡*Cooperative Cosponsorship*

3:40 CATL 56. Kinetic and isotopic consequences of proton-coupled electron transfer events during carbonyl and phenolic compound hydrogenation at protic solvent-transition metal interface. **J. Shangguan**, Y. Chin

4:20 CATL 57. Two-dimensional models for surface science studies of zeolites. **J.A. Boscoboinik**

5:00 CATL 58. Catalysis on singly dispersed Rh atoms anchored on an inert support. **F. Tao**, S. Zhang, Y. Tang

5:40 CATL 59. Modeling molecular water oxidation catalysts at interfaces. **M. Ahlquist**, S. Zhan

Section B
Hampton Inn & Suites Convention Center
Riverside I

Control of Zeolite Structure, Composition & Sites for Catalysis
Cosponsored by INOR
S. Goel, R. Gounder, W.F. Schneider, *Organizers, Presiding*

1:00 CATL 60. Molecular modeling within zeolite catalysis: The methanol-to-olefin process as a case study. **V. Van Speybroeck**

1:40 CATL 61. Diversification of hierarchical two-dimensional zeolite structures for catalysis applications. **D. Liu**, S. Oh, J. Zhang

2:00 CATL 62. Experimental perspectives on controlling desired properties in zeolite materials through synthesis. **S.I. Zones**

2:40 CATL 63. Tailored hierarchical pore structures of beta zeolites through PDA-assisted base leaching. **S. Fernandez**, M. Ostraat, K. Zhang

3:00 Intermission.

3:15 CATL 64. Acid-catalyzed and radical-mediated pathways in condensation and β-scission reactions of oxygenates on aluminosilicates. S. Herrmann, **E. Iglesia**

3:55 CATL 65. New SAPO-based nanoporous materials and some potential applications. **R.L. Bedard**

4:15 CATL 66. The role of isolated Ga cations in MFI on the dehydrogenation of propane and the oligomerization of propene in Ga/H-MFI. **A.T. Bell**

4:55 CATL 67. Towards rational design of Cu/SSZ-13 selective catalytic reduction catalysts: Implications from atomic-level understanding of hydrothermal stability. **F. Gao**, J.M. Song, Y. Wang, E.D. Walter, N. Washton, D. Mei, L. Kovarik, M. Engelhard, S. Prodinger, Y. Wang, C.H. Peden

Section C
Hampton Inn & Suites Convention Center
Riverside III

Machine Learning for Catalysis Research
Cosponsored by CINF and COMP
J.R. Kitchin, H. Xin, *Organizers*
A. Peterson, *Organizer, Presiding*
H.J. Kulik, Z. Ulissi, *Presiding*

1:00 CATL 68. Development of efficient and accurate machine-learning potentials for the simulation of complex catalyst materials. **N. Artrith**

1:40 CATL 69. Towards spectroscopic accuracy in molecular dynamics simulations with machine-learned CCSD(T) force fields. **S. Chmiela**, H.E. Sauceda, K. Müller, A. Tkatchenko

2:00 CATL 70. Global minimization and energy landscape of metal nanoclusters from first principles. **D. Jiang**

2:20 CATL 71. Exploring metal cluster catalysts with DFT based high dimensional neural network potentials. **P. Sautet**, G. Sun

2:40 CATL 72. Machine learning based atomistic force fields. **R. Ramprasad**

3:10 Intermission.

3:30 CATL 73. Machine-learning assisted optimization algorithms for the accelerated development of transferable coarse-grained models. **S. Deshmukh**

3:50 CATL 74. Calculating the potential energy surface and extracting information from it about the dynamics of the system: From neural network potentials to automated reaction pathway determination. **S. Goedecker**

4:20 CATL 75. Machine learnt models for materials design. **S. Sankaranarayanan**

4:50 CATL 76. A review of machine learning strategies for molecular modeling. **L.E. Achenie**

5:10 CATL 77. Prediction of DFT-derived point-charges using machine-learning. **P. Bleiziffer**, S. Riniker

Section D
Hampton Inn & Suites Convention Center
Bienville

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Cosponsored by COMP, ENFL and PHYS
K. Schwarz, R. Sundararaman, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CATL 78. Insights into electrochemical double layer structure at Co/electrolyte interfaces from in situ magnetic characterizations. **P. Allongue**, F. Maroun

1:45 CATL 79. Large-scale simulations of solid-liquid interfaces under realistic electrochemical conditions for energy conversion and storage. **I. Dabo**

2:25 CATL 80. Band alignment at solid-liquid interfaces and nanoplasmonic photocatalysis. **J. Lischner**, L. Blumenthal, P. Tangney, J. Kahk, R. Sundararaman

3:05 Intermission.

3:20 CATL 81. Continuum approaches in electrochemistry: methods, and applications of ENVIRON. **O. Andreussi**

3:40 CATL 82. First-principles interpretations of X-ray spectroscopy at electrochemical interfaces. **D. Prendergast**

4:20 CATL 83. Integrating first principles theory and X-ray reflectivity measurements to determine solid/liquid interfacial structure. **K. Letchworth-Weaver**

4:40 CATL 84. Potential-dependent water structure and dynamics at the hematite-electrolyte interface. **M.E. McBriarty**, J. Stubbs, G.F. von Rudorff, J. Blumberger, E.J. Bylaska, P.J. Eng, K. Rosso

Section E
Hampton Inn & Suites Convention Center
Fulton

Magnetically Recoverable Catalysts
Cosponsored by COLL, ENFL and INOR
L. Bronstein, A.H. Moores, *Organizers*
O. Reiser, *Presiding*

1:00 Introductory Remarks.

1:05 CATL 85. Nanocatalysts embedded in magnetic, microporous polymer platforms: Synthesis and applications. **O. Reiser**

1:40 CATL 86. Benign-by-design preparation of catalytically active magnetically separable nanomaterials. **R. Luque**, A. Balu

2:10 CATL 87. Greener pathways to organics: Sustainable applications of magnetic nanocatalysts. **A.H. Moores**, R. Hudson, M. Masnadi, A. Li

2:40 Intermission.

2:55 CATL 88. Magnetic and carbonaceous nano-catalysts in sustainable chemical transformations. **R.S. Varma**

3:30 CATL 89. Studying corrosion and galvanic reactions of Fe-based nanoparticle catalysts using in situ X-ray absorption spectroscopy. **R.W. Scott**, Y. Yao, Y. Hu

4:00 CATL 90. Silica based magnetically retrievable nanocatalysts for various chemical transformations. **R. Gaur**

4:20 CATL 91. Double-shelled nanoreactor as support for confined catalytic reactions. **G. Arora**

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Challenge & Opportunity in Lignin Valorization
Cosponsored by ENFL, ENVR, INOR and PHYS
F. Wang, *Organizer*
M.M. Abu-Omar, G. Beckham, *Organizers, Presiding*

1:00 CATL 92. Oxidation methods for lignin conversion into low molecular-weight aromatics. **S.S. Stahl**

1:20 CATL 93. Valorization of grass lignins: Swift and selective recovery of pendant aromatic groups with ozone. A.M. Danby, M. Lundin, J.R. Silverman, **B. Subramaniam**

1:40 CATL 94. Adventures in lignin oxidation. **N.J. Westwood**

2:00 CATL 95. Catalytic beta-O-4 ether cleavage in lignin and lignin models by selective activation, cleavage and scavenging. C. Lancefield, R. Jastrzebski, L. Teunissen, K. Khalili, A. Martinez Pascual, B. Weckhuysen, **P. Bruijnincx**

2:20 Intermission.

2:30 CATL 96. Redox catalysis strategies for biomass conversion. **C. Stephenson**

2:50 CATL 97. Catalytically oxidative cleavage of lignin C-C bond. **F. Wang**

3:10 CATL 98. A comparative study on oxidative approaches for lignin depolymerization. **Y. Song**, J.K. Mobley, J. Ralph, M. Crocker

3:30 CATL 99. Valorizing lignin by base and metal catalysis. **C. Bolm**

3:50 CATL 100. Toward the oxidative deconstruction of lignin: Oxidation of β-1 and β-5 linkages. **Z. Fang**, M.S. Meier, M. Crocker

Synthetic Chemistry Addressing Challenges in Energy & the Environment
Sponsored by INOR, Cosponsored by CATL and WCC

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

Carbon Dioxide Conversion & Artificial Photosynthesis
Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

MONDAY MORNING

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces

Theory

Cosponsored by COLL, ENVR and PHYS
S. Laursen, A. Savara, *Organizers*
L. Baker, *Organizer, Presiding*

8:00 CATL 101. A new mechanism for the oxidative coupling of methane: Experiment and theory in concert. **J. Sauer**

8:40 CATL 102. Selectivity control for alcohol amination with ammonia. **P. Sautet**, T. Wang, J. Ibanez, M. Sabbe, C. Michel, M. Pera-Titus, P. Sebastien

9:20 CATL 103. Selective catalysts for higher alcohol synthesis: A combined DFT and micro-kinetic modeling study. **J. Schumann**, P. Bothra, F. Abild-Pedersen, J.K. Norskov

9:40 Intermission.

10:00 CATL 104. Surrogate model accelerated mechanism discovery. **T. Bligaard**

10:40 CATL 105. The role of surface chemical reactivity towards atomic hydrogen in the activation and cleavage of C-H and O-H bonds for dehydrogenation and reforming over intermetallic compounds. Y. He, Y. Song, **S. Laursen**

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11:20 CATL 106. Equilibrium constants and rate constants for adsorbates in microkinetic modelling: 2D gas, 2D lattice gas, and hindered translator models. **C.T. Campbell**, L. Arnadottir

11:40 CATL 107. Benchmark first-principles calculations of adsorbate free energies. **W.F. Schneider**, A. Bajpai, P. Mehta, K. Frey

Section B
Hampton Inn & Suites Convention Center
Riverside I/II

Challenge & Opportunity in Lignin Valorization
Cosponsored by ENFL, ENVR, INOR and PHYS
M.M. Abu-Omar, *Organizer*
G. Beckham, F. Wang, *Organizers, Presiding*

8:00 CATL 108. Biomass-derived polymers incorporating hydroxycinnamates. **A.M. Kasko**, B. Upton

8:20 CATL 109. Lignin extraction and catalytic upgrading from genetically modified poplar. **M.M. Abu-Omar**, H. Luo

8:40 CATL 110. Partial delignification of biomass for recovery of hydroxycinnamic acids as a "lignin first" strategy. **R. Brown**

9:00 CATL 111. An integrated, flexible biorefinery process based on formic acid. **N. Yan**

9:20 Intermission.

9:30 CATL 112. Seeing the wood for the trees: Taking a new look at lignin nitrosation. **R. Baker**

9:50 CATL 113. An overview of lignin disassembly with Cu-doped porous metal oxides. **J.A. Barrett**, P.C. Ford, C.M. Bernt, M.A. Chui, C. Stickelmaier

10:10 CATL 114. Catalytic transformation of lignin into aromatics under visible-light irradiation. X. Wu, S. Xie, J. Lin, Q. Zhang, W. Deng, **Y. Wang**

10:30 CATL 115. Making single monomeric building blocks from lignin and theri further conversion into useful products. **J.G. De Vries**, E. Lanfranchi, P.J. Deuss, D. Janssen, K. Barta

10:50 CATL 116. Role of catalysis in a lignin-first biorefinery. **B.F. Sels**

Section C
Hampton Inn & Suites Convention Center
Riverside III

Machine Learning for Catalysis Research
Cosponsored by CINF and COMP
A. Peterson, H. Xin, *Organizers*
J.R. Kitchin, *Organizer, Presiding*
H.J. Kulik, A. Medford, *Presiding*

8:00 CATL 117. SchNet: A continuous-filter convolutional neural network for modeling quantum interactions. **K.T. Schütt**, P. Kindermans, H.E. Sauceda, S. Chmiela, A. Tkatchenko, K. Müller

8:20 CATL 118. Withdrawn

8:40 CATL 119. Development and analysis of "surrogate" hybrid functionals using neural networks, uncertainty quantification, and visualization. **A.J. Medford**, X. Lei, P. Chau, F.M. Hohman

9:00 CATL 120. Identification of systematic DFT-errors and uncertainty estimation in catalyst design using machine learning. **T. Vegge**, R. Christensen, C.F. Dickens, H.A. Hansen

9:20 CATL 121. Quantum machine learning. **O. von Lilienfeld**

10:00 Intermission.

10:20 CATL 122. Machine learning enabled local energies. **B. Hammer**

10:50 CATL 123. Accelerating routine atomistic calculations. **A. Peterson**

11:20 CATL 124. Applications of machine learning for studying local solvation environments. M. Groenonboom, S. De, M. Ceriotti, **J.A. Keith**

11:40 CATL 125. Combined *ab initio* and machine learning approaches for modeling catalyst-water interfaces. **A. Kolpak**

Section D
Hampton Inn & Suites Convention Center
Bienville

Operando Techniques for Catalytic & Photocatalytic Fuel Conversion Studies
Cosponsored by ENFL
M. Liu, *Organizer*
C. Wang, *Organizer, Presiding*

8:00 CATL 126. The dynamic structure of catalysts under ambient conditions: From characterization to stabilization of active ensembles. **D.J. Stacchiola**

8:40 CATL 127. Instrumentation of in situ/operando studies of catalysts. **F. Tao**

9:20 CATL 128. Interaction of acid gas with faceted metal oxide catalysts. **S. Luo**, Z. Wu

9:45 Intermission.

9:55 CATL 129. High spatial resolution mapping of catalytic reactions on single nanoparticles. **E. Gross**

10:35 CATL 130. *Operando* XAFS study of Au/C catalysts for acetylene hydrochlorination reaction. G. Malta, S. Freakley, S. Kondrat, L. Lu, E. Gibson, P. Wells, C. Kiely, **G. Hutchings**

11:15 CATL 131. Promoting the ethylene yield in ethane oxidative dehydrogenation reaction over Mo_2C catalyst via oxygen modification. **S. Yao**, B. Yan, J.G. Chen

11:40 CATL 132. In-situ/operando characterization of supported Ir single atoms. Y. Lu, A. Hoffman, A. Boubnov, S.R. Bare, **A.M. Karim**

Section E
Hampton Inn & Suites Convention Center
Fulton

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Cosponsored by ENFL, INOR and PHYS
C.A. Carrero, R.B. Getman, I. Hermans, *Organizers, Presiding*

8:00 CATL 133. Methane steam reforming: Using external electric fields to enhance the catalytic performance of Ni. F. Che, J.T. Gray, S. Ha, **J. McEwen**

8:30 CATL 134. Activation of light hydrocarbons by catalysts supported on metal-organic framework nodes. **C.J. Cramer**

8:50 CATL 135. On the dynamic nature of Mo sites for methane dehydroaromatization. **I. Vollmer**, J. Gascon, F. Kapteijn, I. Yarulina, A.I. Olivos Suarez, B. van der Linden, Y.G. Sneider

9:10 CATL 136. Critical surface parameters for the oxidative coupling of methane over Mn-Na-W/SiO_2 catalyst. N. Hayek, N. Lucas, C. Warwar Damouny, **O. Gazit**

9:30 Intermission.

9:50 CATL 137. Computational studies of the oxidation of C1 and C2 alkanes to alcohols using metal-organic frameworks. M. Barona, H.A. Doan, P. Liao, P. Miro, R.B. Getman, O.K. Farha, J.T. Hupp, **R. Snurr**

10:10 CATL 138. Niobium promotion of nickel oxide catalsyts for ethane oxidative dehydrogenation to ethylene. A.E. Diaz-Alvarez, F. Rubio-Marcos, J.F. Fernandez, **M.A. Banares**

10:40 CATL 139. Effect of Mo content in methane dehydroaromatization using sulfated zirconia supported Mo_2C catalysts. **S. Kanitkar**, A. Abedin, S. Bhattar, J.J. Spivey

11:00 CATL 140. Multi-physics numerical modeling of multi-phase flow and heat transfer for smart catalyst reactor. **M. Zaidani**, M. Jouiad, M. Sanduleanu, M.B. Sassi

11:20 CATL 141. Investigating the kinetics of supported, Pincer-ligated iridium catalysts in a continuous-flow gas phase system for C_4 upgrading. **B. Sheludko**, M.T. Cunningham, A.S. Goldman, F.E. Celik

11:40 CATL 142. Development of descriptors for methane-to-methanol conversion and side-reactions on zeolite-supported tri-metal tri-oxo catalysts. **N.K. Dandu**, S.O. Odoh

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Cosponsored by COMP, ENFL and PHYS
K. Schwarz, R. Sundararaman, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 143. Local probes at the Pt(hkl)/electrolyte interface. **J.M. Feliu**

8:45 CATL 144. Beyond the point charge scheme in the description of charge polarization at electrochemical interfaces. **S. Sakong**, A. Gross

9:05 CATL 145. Electric fields, solvation, protonation, and frustration at electrochemical interfaces probed by vibrational spectroscopy. J. Patrow, S.A. Sorenson, **J. Dawlaty**

9:45 CATL 146. Recent developments in modelling the electrochemical interface. **K. Chan**

10:05 Intermission.

10:20 CATL 147. Modeling chemisorption at electrochemical interfaces from first principles. **P. Sautet**

11:00 CATL 148. Carbon monoxide and water coadsorption on platinum and platinum-based mixed-metal anode catalysts for polymer electrolyte membrane fuel cells. **N. Dimakis**, M.J. Farooqi, I. Salas, L. Gonzalez, E.S. Smotkin

11:20 CATL 149. First-principles investigation of adsorbed hydrogenated N-heterocycles as hydride shuttles for catalytic CO_2 reduction on p-GaP photoelectrodes. **M. Lessio**, T.P. Senftle, E.A. Carter

11:40 CATL 150. Electrifying model catalysis: Complex model catalysts studied in ultrahigh vacuum and under electrochemical conditions. **J. Libuda**

Computational Catalyst Design for Energy Conversion & Storage

Advances in Theory, Computational Models & Approaches

Sponsored by COMP, Cosponsored by CATL and CINF

Carbon Dioxide Conversion & Artificial Photosynthesis

Theoretical Studies, Policy & Catalytic Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

MONDAY AFTERNOON

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

1:00 CATL 151. Size, support, and alloy effects on cluster catalysis. T.J. Gorey, E.T. Baxter, A.C. Cass, **S.L. Anderson**

1:40 CATL 152. Visualizing interfacial chemical kinetics and dynamics using supersonic molecular beams and In situ scanning tunneling microscopy. **S.J. Sibener**, R. Edel, T. Grabnic, B. Wiggins, L. Avila-Bront

2:20 CATL 153. Surface electron dynamics in CuFeO2 catalysts studied by ultrafast XUV spectroscopy. **L. Baker**

3:00 CATL 154. Electronic structure and reactivity of cluster-based nanocatalysts. **M.G. White**, M. Xue, K.R. Goodman, Y. Ma, S. Liu, P. Liu

3:40 Intermission.

4:00 CATL 155. Withdrawn

4:40 CATL 156. Model studies in energy-related catalysis and electrocatalysis. **J.**

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Libuda

5:20 CATL 157. Acetol adsorption and reactivity on metal single crystals and oxide films: From UHV conditions to mTorr range. **F.C. Calaza**, O. Karslioglu, H. Bluhm, M. Sterrer, H. Freund

5:40 CATL 158. NO+CO oxidation on Pd(100) studied by ambient-pressure XPS. **O. Karslioglu**, A.R. Head, T. Gerber, J. Raso, L. Trotochaud, Y. Yu, P. Kerger, H. Bluhm

Section B
Hampton Inn & Suites Convention Center
Riverside I/II

Homogeneous Catalysis for Applied Organic Synthesis
Cosponsored by INOR and ORGN‡
T. Colacot, B.H. Lipshutz, *Organizers*
S. Chandrasekaran, S. Trice, *Presiding*

1:00 Introductory Remarks.

1:15 CATL 159. Nobel Keynote: Fast and practical Pd catalyzed cross-coupling of organolithium reagents. **B. Feringa**

2:10 CATL 160. Discovery and development of novel chromium-based catalysts for ethylene tetramerization. **M.S. Rosen**, S. Boelter, D. Davies, J. Klosin, K. Milbrandt, D. Mort, A. Smith, D. Welsh, D. Wilson, M. Wiltzius

2:45 CATL 161. Structure activity relationship of homogeneous catalysts in organic synthesis. **T. Colacot**

3:20 Intermission.

3:40 CATL 162. Werner complexes: A new class of chiral hydrogen bond donor catalysts for enantioselective organic reactions. **J.A. Gladysz**

4:15 CATL 163. Synthetic organic chemistry in water. Faster, better, cheaper. **B.H. Lipshutz**

Section C
Hampton Inn & Suites Convention Center
Riverside III

Machine Learning for Catalysis Research
Cosponsored by CINF and COMP
J.R. Kitchin, A. Peterson, *Organizers*
H. Xin, *Organizer, Presiding*
A. Medford, Z. Ulissi, *Presiding*

1:00 CATL 164. Determining physical/chemical properties for material systems with data mining. **H. Dam**, T. Pham, H. Kino, K. Terakura, T. Miyake

1:20 CATL 165. Utilizing limited training data in materials informatics. **C. Ling**

1:40 CATL 166. Machine learning surrogate models. **J. Boes**

2:00 CATL 167. The role of transfer in reaction development. **P.M. Zimmerman**

2:30 CATL 168. Using machine-learning to create predictive material property models. **C. Wolverton**

3:10 Intermission.

3:30 CATL 169. Machine learning and statistical analysis for materials science: Stability and transferability of fingerprint descriptors and chemical insights. **U.V. Waghmare**, P. Pankajakshan, S. Sanyal, O. deNoord, I. Bhattacharya, A. Bhattacharyya

3:50 CATL 170. Finding patterns, correlations, and descriptors in materials data using subgroup discovery and compressed sensing. **B.R. Goldsmith**, C. Bartel, M. Boley, C. Sutton, J. Vreeken, C. Musgrave, R. Ouyang, L.M. Ghiringhelli, M. Scheffler

4:20 CATL 171. Adaptive molecular property estimator using convolutional neural networks. **K. Han**, C. Coley, W.H. Green

4:40 CATL 172. Machine learning-based structure recognition for automated reactivity predictions through transition state calculations. **A. Bochevarov**, L.D. Jacobson, K. Marshall, J. Staker

5:10 CATL 173. Machine learnt meso-scale models. **S. Singh**, K. Bejagam, S. Deshmukh

5:30 CATL 174. Machine-learning frameworks in molecular simulation. **J.R. Kitchin**

Section D
Hampton Inn & Suites Convention Center
Bienville

Operando Techniques for Catalytic & Photocatalytic Fuel Conversion Studies
Cosponsored by ENFL
C. Wang, *Organizer*
M. Liu, *Organizer, Presiding*

1:00 CATL 175. Dynamical measurements of surface layers in water-splitting photocatalysts. **M. Sfeir**

1:40 CATL 176. Operando measurements of water oxidation intermediates on metal oxide semiconductor electrodes. **T. Hamann**

2:20 CATL 177. Interaction of Water with an Ultrathin ZnO Layer. **J. Lee**

3:00 Intermission.

3:10 CATL 178. In-situ methods for probing electrocatalytic reactions at metal and metal oxide nanostructures. **D.J. Fermin**, V. Celorrio

3:50 CATL 179. Synchrotron-based *In situ* characterization of nanostructured electrocatalysts for clean-energy applications. **K. Sasaki**, N. Marinković, R.R. Adzic

4:30 CATL 180. Anomalous conductivity tailored by domain boundary transport in crystalline $BiVO_4$ photoanodes. **W. Zhang**, D. Yan, J. Li, Q. Wu, J. Cen, L. Zhang, A. Orlov, H. Xin, J. Tao, M. Liu

4:55 CATL 181. Operando structural investigation of epitaxial iron gropup metal oxide thin films as OER catalysts. **P. Allongue**, F. Maroun, F. Reikowski, I. Pacheco-Bubi, T. Wiegmann, J. Stettner, O. Magnussen

Section E
Hampton Inn & Suites Convention Center
Fulton

Magnetically Recoverable Catalysts
Cosponsored by COLL, ENFL and INOR
A.H. Moores, *Organizer*
L. Bronstein, *Organizer, Presiding*
E. Rebrov, *Presiding*

1:00 CATL 182. Enhanced thermal stability of silica-coated magnetite nanoparticles for the desing of advanced catalysts. **L.M. Rossi**, L. Vono, J.R. Matos, R. Landers, S. Masunaga, R. Jardim

1:35 CATL 183. Three-in-one functional magnetic catalysts: Fast heating, mixing and separation in gas-liquid reactions. **E. Rebrov**

2:05 CATL 184. Thermal plasma synthesis and characterization of hybrid spinel nanoferrites for catalysis. **N. Braidy**, N. Dumaresq, S. Bastien, A.H. Moores

2:35 Intermission.

2:50 CATL 185. Magnetically recoverable catalysts: Magnetic support influences catalysis. **L. Bronstein**

3:20 CATL 186. Withdrawn

3:50 CATL 187. Catalytic activity of anisotropic magnetic nanoparticles activated via RF induction heating. **N. da Silva Moura**, J. Bursavich, H. Simonson, C. Boudreaux, J.A. Dorman

4:10 CATL 188. A bottle-around-a-ship method to generate hollow thin-shelled particles containing encapsulated iron species with application to the environmental decontamination of chlorinated compounds. V.T. John, **Y. Su**

4:30 CATL 189. Synthesis of ionic liquid supported silica-coated magnetic nanocatalyst for the straightforward one-pot synthesis of bioactive *N*-aryl oxazolidin-2-ones. **R. Gupta**, R.K. Sharma

4:50 Concluding Remarks.

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Cosponsored by ENFL, INOR and PHYS
C.A. Carrero, R.B. Getman, I. Hermans, *Organizers, Presiding*

1:00 CATL 190. Precise deposition of Pt promoter onto silica supported cobalt for Fischer-Tropsch synthesis. F. Almalki, J.R. Monnier, **J.R. Regalbuto**

1:40 CATL 191. Screening hydrocarbon activation pathways with computational alchemy. K. Saravanan, **J.A. Keith**

2:00 CATL 192. Methane activation and conversion via reforming using nonconventional catalysts and conditions. U. Cimenler, N. Elsayed, D. Maiti, Y. Sokefun, B. Joseph, **J. Kuhn**

2:20 CATL 193. On the unusual redox cycle at the vanadia ceria interface and its relevance for ethane ODH. A. Iglesias-Juez, M.V. Martinez-Huerta, E. Rojas-Garcia, J. Jehng, **M.A. Banares**

2:45 Intermission.

3:00 CATL 194. Immobilization of earth abundant metals coordinated in heterobimetallic ligand scaffolds on metal organic frameworks (MOFs). **J. Vitillo**, K. Riley, S.P. Desai, Z. Garr, A. Platero-Prats, J. Zheng, M. Simons, T. Webber, K.W. Chapman, D.M. Camaioni, O. Farha, J.T. Hupp, R. Penn, C. Lu, L. Gagliardi

3:20 CATL 195. Mechanistic approach to probe ligand-dependence of CH activation kinetics in bioinspired dicopper complexes. **S. Mallikarjun Sharada**

3:40 CATL 196. Reactivity and selectivity descriptors for oxidative dehydrogenation of small hydrocarbons and oxygenates on metal oxides. **P. Deshlahra**, E. Iglesia

4:00 CATL 197. Computational design of active and selective catalyst for methane conversion to value-added products. **S. Wang**, L. Grabow

4:20 CATL 198. Au(III) complexes catalyze direct partial oxidation of methane at low temperature in ionic liquids. **T. Huang**, Z. Xu, P. Yan, X. Liu, **Z. Zhang**

4:40 CATL 199. Conversion of methane to methanol and ethanol in a single reactor. C. Okolie, Y. Lyu, L. Kovarik, E. Stavitski, **C. Sievers**

Computational Catalyst Design for Energy Conversion & Storage

Development of Electro- & Photocatalysts

Sponsored by COMP, Cosponsored by CATL and CINF

Carbon Dioxide Conversion & Artificial Photosynthesis
Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
A. Savara, *Organizer*

8:00–10:00

302, 304, 310, 315, 317, 319-321, 323, 331, 334, 337, 340, 346, 350, 352-353. See subsequent listings.

TUESDAY MORNING

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Cosponsored by COLL, ENVR and PHYS
S. Laursen, A. Savara, *Organizers*
L. Baker, *Organizer, Presiding*

8:00 CATL 200. Mechanistic studies of CO and benzyl alcohol oxidation over Au: Roles of support, proton transfer, and water. **B.D. Chandler**

8:40 CATL 201. Mechanisms of low-temperature oxidation and H_2 photoproduction from water using Au-TiO_2 catalysts. **F. Zaera**

9:20 CATL 202. Kinetics and mechanism of aspartic acid decomposition on chiral

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Cu{*hkl*}$^{R\&S}$ surfaces. **A.J. Gellman**, P. Kondratyuk, Y. Yun, A. Reinicker, S. Dutta

10:00 Intermission.

10:20 CATL 203. N-heterocyclic carbene molecules (NHCs) as chemical markers for high spatial resolution mapping of catalytic reactions on surfaces. S. Deri, **E. Gross**

10:40 CATL 204. Enhanced activity and selectivity on the surface of ordered bimetallic catalysts. **W. Huang**, R. Maligal Ganesh, Y. Pei, Z. Qi

11:20 CATL 205. Catalyst architecture for stable, atomically dispersed Pt-group metals enables mechanistic analysis of reactivity. **P. Christopher**

Section B
Hampton Inn & Suites Convention Center
Riverside I

Homogeneous Catalysis for Applied Organic Synthesis
Cosponsored by INOR and ORGN‡
T. Colacot, B.H. Lipshutz, *Organizers*
G. Grasa, I. Ibnusaud, *Presiding*

8:50 Introductory Remarks.

8:55 CATL 206. First row transition metal catalysts for synthesis and radiolabeling of active pharmaceutical ingrediants. **P.J. Chirik**

9:30 CATL 207. Alkylphosphine cyclometallation as a mode of catalyst deactivation and a source of active catalysts. **K.H. Shaughnessy**

10:05 Intermission.

10:25 CATL 208. Pincer iridium complexes for oxidations and reductions. B. Bark, J.M. Goldberg, S. Rubashkin, A.M. Wright, Z. Syed, D.M. Heinekey, **K.I. Goldberg**

11:00 CATL 209. Nobel Keynote: Selective olefin metathesis catalysis in synthesis. **R.H. Grubbs**

Section C
Hampton Inn & Suites Convention Center
Riverside III

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Cosponsored by ENFL, ENVR and INOR
J. Choi, O. Gazit, M. Kidder, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CATL 210. Tuning pore hierarchy and acidity of heterogeneous catalysts for biomass conversion. **K. Wilson**

8:35 CATL 211. Investigation of nickel, cobalt, and iron oxyhydroxide anodes for the electrochemical oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid. **B.J. Taitt**, D. Nam, K. Choi

8:50 CATL 212. Determination of surface structure of ReOx-Pd/CeO2 for improved deoxydehydration of organic compounds. **E. Barrow**, S. Sanchez, J. Lauterbach

9:05 CATL 213. Selective hydrogenation of γ-valerolactone to pentanoic acid over Pt/zeolite using formic acid as a hydrogen source. **M. Al-Naji**, J. Van Aelst, N. Wilde, R. Glaeser, B.F. Sels

9:20 CATL 214. 1-hydroxy-hexane-2,5-diketone as an interesting new platform chemical. **J.G. De Vries**, B. Wozniak, S. Hinze, Y. Li, A. Spannenberg

9:35 Intermission.

9:50 CATL 215. Role of heterogeneous catalysis in biomass conversion. **B.F. Sels**

10:20 CATL 216. Fundamental investigation of electrocatalytic low temperature bio-oil stabilization. **A. Padmaperuma**, S. Akhade, D.C. Cantu, R. Rousseau, V. Glezakou, M. Lilga, J. Holladay

10:35 CATL 217. Renewable acrylonitrile enabled via catalytic nitrilation chemistry. **E. Karp**, T. Eaton, V. Sànchez i Nogué, V. Vorotnikov, L. Manker, D. Brandner, W. Michener, G. Beckham

10:50 CATL 218. Hydrogenation of biomass based furans to fine chemicals through homogeneous Ir catalysis. **Z. Xu**, Z. Zhang

11:05 CATL 219. Catalytic conversion of ethanol to butadiene: A detailed DFT investigation of the complex reaction mechanism. **V. Butera**, Y. Choe, Y. Tanabe, T. Miyazawa, T. Fujitani

11:20 CATL 220. Synthesis of glycerol carbonate from CO_2 using metal oxide catalysts. **C.J. Mota**, L. Ozório

Section D
Hampton Inn & Suites Convention Center
Bienville

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Cosponsored by COMP and ENFL
A. Savara, *Organizer*
V.G. Baldovino-Medrano, J.J. Bravo-Suarez, *Organizers, Presiding*

8:00 CATL 221. Some considerations in the development and scale to commercial level for zeolites as catalyst components. **S.I. Zones**

8:40 CATL 222. Scale-up, evaluation and commercialization of a novel family of FCC catalysts. **J. Garcia Martinez**, N. Linares, E. De Oliveira Jardim, E. Serrano

9:05 CATL 223. Novel catalytic approach towards C4 olefins and gasoline octane in fluid catalytic cracking. **Y. Shu**, E. Yik, M. Ziebarth, B.H. Cipriano, W. Cheng

9:30 CATL 224. Key factors for industrial fluid catalytic cracking catalyst evaluations. **W.E. Alvarez**

9:55 Intermission.

10:15 CATL 225. Mass transfer limitations occurring during the scaling-up of a NiMoP/γAl_2O_3 hydrotreatment catalyst. **R.A. Prada Silvy**

10:40 CATL 226. Characterization of spent catalysts from an industrial hydrotreating unit give insight upon catalyst life evolution. **L.J. Duarte**, L.L. Garzón, **V.G. Baldovino-Medrano**

11:05 CATL 227. *In situ* catalytic fast pyrolysiss (CFP) and hydrotreating to convert biomass to fuel blendstocks: Scale-up production of CFP catalyst and scale-up in situ CFP testing. **H. Wang**, F.A. Agblevor, C. Lindfors

11:30 CATL 228. Catalytic upgrading of pyrolysis oil. **M.V. Olarte**, D.C. Elliott, A.H. Zacher, S.B. Jones, A. Padmaperuma, D. Stephenson, C. Drennan

Section E
Hampton Inn & Suites Convention Center
Fulton

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Cosponsored by ENFL, INOR and PHYS
C.A. Carrero, R.B. Getman, I. Hermans, *Organizers, Presiding*

8:00 CATL 229. Boron-based catalysts for the oxidative dehydrogenation of propane. **I. Hermans**

8:30 CATL 230. Mechanistic study of oxidative C-H and C-C bond cleavage of ethane. **S. Kattel**, J.G. Chen, P. Liu

8:50 CATL 231. Uniform Pt/Pd bimetallic nanocrystals demonstrate platinum effect on palladium methane combustion activity and stability. **E.D. Goodman**, S. Dai, A. Yang, C. Wrasman, A. Gallo, S.R. Bare, A. Hoffman, T.F. Jaramillo, G. Graham, X. Pan, M. Cargnello

9:10 CATL 232. Selective oxidation of n-butane to 1-butanol over transition metal catalysts encapsulated by metal-organic frameworks. **J. Zhu**, R.B. Getman

9:30 Intermission.

9:40 CATL 233. Aldol condensation on oxide catalysts: Mechanisms and effects of thermal treatments and metal identity. **D. Flaherty**

10:10 CATL 234. *In-situ* elucidation of the active state of Co-CeO_x catalysts in the dry reforming of methane: The important role of the reducible oxide support and interactions with cobalt. **F. Zhang**, J. Rodriguez, S.D. Senanayake, T. Kim, Z. Liu

10:30 CATL 235. Predicting low-temperature methane activation via doped metal oxides from first principles. **V. Fung**, F. Tao, D. Jiang

10:50 CATL 236. Improving conversion and hydrogen efficiency for propylene epoxidation. **Z. Lu**, C.H. Turner, Y. Lei

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Enabling Fundamental Advances in Catalysis & Surface Science

Cosponsored by ENVR, INOR and PHYS
W.O. Gordon, *Organizer*
M.L. McEntee, J. Pietron, *Organizers, Presiding*
W. Gordon, *Presiding*

8:00 CATL 237. Structure and activity of Pd on Ag(111) for hydrogen activation: Modeling catalyst materials under ambient pressure. **C.M. Friend**

8:30 CATL 238. Mechanistic studies of CO/CO_2 reactivity over inverse (oxide/metal) model catalysts. **R.M. Palomino**, S.D. Senanayake, J. Rodriguez

8:55 CATL 239. Pd doped $CaCo_xZr_{1-x}O_{3-\delta}$ novel perovskites for automotive emissions control. **Q. Zheng**, M.A. Lail

9:15 CATL 240. Unlocking active sites for formaldehyde oxidation on manganese oxide catalyst. **K. Akkiraju**, Y. Shao-Horn, D. Weinberger, W.F. Ruettinger

9:35 CATL 241. Ultrathin two-layered anatase nanosheets as prospective catalysts and catalyst support. **A.V. Vorontsov**, G. Lyubas

9:55 Intermission.

10:10 CATL 242. In situ analysis of the chemistry of environmental interfaces. **V.H. Grassian**

10:40 CATL 243. *Operando* Raman-online FTIR investigation on the role of vanadium and gold doping on ceria-based catalysts for toluene elimination. **M.A. Banares**, Q. Wang, W. Chen, K. Yeung

11:10 CATL 244. Total methanol oxidation studied by MS-DRIFT operando and MES on bimetallic Au-Pd catalysts. **F.C. Calaza**, A. Baldó, C. Olmos, X. Chen, S. Collins

11:30 CATL 245. Catalytic ozonation of phenol via GO/MgO nanocomposites. **M. Heidarizad**, A. Quicksall

Computational Catalyst Design for Energy Conversion & Storage

Development of Homogeneous & Heterogeneous Catalysts

Sponsored by COMP, Cosponsored by CATL and CINF

Carbon Dioxide Conversion & Artificial Photosynthesis

Photocatalytic Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

TUESDAY AFTERNOON

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

1:00 CATL 246. Spectroscopic characterization of reaction pathways over a Pd-Cu(111) single-atom alloy. C. Kruppe, J. Krooswyk, **M. Trenary**

1:40 CATL 247. Inverse oxide/metal catalysts and the study of reaction mechanisms. **J. Rodriguez**

2:00 CATL 248. Methane activation in dry reforming over metal oxide supported Ni nanoparticles: role of support reducibility on low temperature dry reforming. M. Li, J. Carey, A. Van Veen, **M. Nolan**

‡*Cooperative Cosponsorship*

2:20 CATL 249. Methane activation on metal oxide catalysts: Importance of site confinement. **P. Liu**, Z. Zuo, S. Liu, J. Rodriguez

3:00 Intermission.

3:20 CATL 250. Elucidating the role of oxygen coverage in CO_2 reduction on Mo_2C. **M. Dixit**, X. Peng, M. Porosoff, H.D. Willauer, G. Mpourmpakis

3:40 CATL 251. Laser-induced oxygen activation probed by machine-learning accelerated nonadiabatic molecular dynamics. J. Wang, **H. Xin**

4:20 CATL 252. Using fast pressure transients to relate mechanistic studies in ultrahigh vacuum to catalytic reactors: Selective oxidation of methanol on nanoporous gold. **R.J. Madix**, C. Reece, E. Redekop

5:00 CATL 253. Elucidation of the anchoring and restructuring mechanisms of metal oxides on silica. **I. Hermans**

5:20 CATL 254. Conversion of alcohols over LaMnO3 and La0.7Sr0.3MnO3 in the presence and absence of oxygen. Y. Zhang, F. Polo Garzon, M. Kidder, D.R. Mullins, **A. Savara**

5:40 CATL 255. Insights into hydrodeoxygenation of phenol on FeMoP, RuMoP and NiMoP bimetallic phosphide catalysts using density functional theory (DFT) study. **V. Jain**, N. Rai

Section B
Hampton Inn & Suites Convention Center
Riverside I

Homogeneous Catalysis for Applied Organic Synthesis

Cosponsored by INOR and ORGN‡
T. Colacot, B.H. Lipshutz, *Organizers, Presiding*

1:00 CATL 256. Nobel Keynote: Magical power of d-block transition metals as exemplified by Pd-catalyzed cross-coupling and Zr-catalyzed carboalumination (ZACA reaction). **E. Negishi**

1:55 CATL 257. Computational chemistry in homogeneous transition metal catalysed reactions: A future prospective. **V. Avasare**, **S. Pal**, P. Jain, D. Das

2:15 CATL 258. Metal catalyzed reactions: Transforming "discoveries" into "potential manufacturing processes" for agrochemical molecules. **J. Oppenheimer**

2:50 Intermission.

3:05 CATL 259. Design, development and execution of a continuous flow enabled API manufacturing route. **J.R. Martinelli**

3:40 CATL 260. Driving synthesis by oxidation. **J. Lumb**

4:15 CATL 261. Nickel-catalyzed reactions of amide derivatives. **N.K. Garg**

4:50 CATL 262. Homogeneous catalysis in applied organic synthesis: A critical evaluation. **S. Chandrasekaran**

5:10 Concluding Remarks.

Section C
Hampton Inn & Suites Convention Center
Riverside III

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels

Cosponsored by ENFL, ENVR and INOR
J. Choi, O. Gazit, M. Kidder, *Organizers, Presiding*

1:00 CATL 263. Valorisation of side-products from furanics conversion: Towards valuable chemicals and advanced catalytic nanomaterials. L. Filiciotto, A. Balu, **R. Luque**

1:30 CATL 264. Utilizing ring-opening tautomerization for the facile catalytic conversion of biomass-derived cyclic hemiacetals and lactones to β,β-diols. **K. Barnett**, Z. Brentzel, Z. Huang, K. Huang, S. Burt, I. Hermans, C. Maravelias, J.A. Dumesic, G.W. Huber

1:45 CATL 265. Tetabutylphosphonium bromide: A versatile ionic liquid catalyst for the biobased production of butadiene and acrylic acid. **M. Stalpaert**, F.G. Cirujano, D. De Vos

2:00 CATL 266. ZrO_2-based catalysts with enhanced hydrothermal stability for the aqueous-phase *In-situ* hydrogenation of levulinic acid. M. Al-Naji, M. Popova, R. Glaeser, **N. Wilde**

2:15 CATL 267. Development of catalytic anodes that enable electrochemical oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid in acidic media. **S.R. Kubota**, K. Choi

2:30 CATL 268. Transesterification of DMC and glycerol catalyzed by Li-La-based catalysts. **L. Yajin**, D. He

2:45 Intermission.

3:00 CATL 269. Titania-encapsulated nickel nanoparticle as catalyst for selective hydrodeoxygenation of guaiacol to phenolics. **X. Zhang**, P. Yan, B. Zhao, K. Liu, **Z. Zhang**

3:30 CATL 270. Kinetics of ethanol dehydrogenation on MgO-SiO_2 mixed oxide catalysts. **H. Abdulrazzaq**, T.J. Schwartz

3:45 CATL 271. Controlling reaction selectivity and boosting reaction rate through the surface termination of perovskite catalysts. **F. Polo Garzon**, S. Yang, V. Fung, G. Foo, E. Bickel, M.F. Chisholm, M. Kidder, D. Jiang, Z. Wu

4:00 CATL 272. Withdrawn

4:15 CATL 273. Withdrawn

4:30 CATL 274. Catalytic properties of molybdenum-based bimetallic phosphides for deoxygenation reactions. Y. Bonita, D.J. Rensel, **J.C. Hicks**

Section D
Hampton Inn & Suites Convention Center
Bienville

Operando Techniques for Catalytic & Photocatalytic Fuel Conversion Studies

Cosponsored by ENFL
C. Wang, *Organizer*
M. Liu, *Organizer, Presiding*

1:00 CATL 275. Au/β-MoC catalyst for the low temperature water gas shift reaction. **D. Ma**

1:40 CATL 276. Colloid-templated porous catalysts for efficient catalysis: CO oxidation using embedded dilute PdAu alloys. **M. Luneau**, T. Shirman, A.C. Filie, A. Stevanovic, J. Timoshenko, E. Shirman, R.J. Madix, A. Frenkel, J. Aizenberg, C.M. Friend

2:20 CATL 277. Scientific data mining in nanoscale visualization of catalysis at work. **Y. Liu**, F. Meirer, B. Weckhuysen, P. Pianetta

3:00 Intermission.

3:10 CATL 278. Atomically engineered gold-copper nanocatalysts for selective CO_2 conversion. **D. Kauffman**, D. Alfonso

3:50 CATL 279. Toward "on the fly" analysis of reactive sites from their X-ray absorption spectra. J. Timoshenko, N. Marcella, **A. Frenkel**

4:30 CATL 280. Developing new catalytic application for selective CO_2 conversion using *in situ* study on doping-segregation mechanism. **J. Cen**, Q. Wu, B. Yan, D. Yan, Y. Zhao, M. Liu, A. Orlov

4:55 CATL 281. Insights into Cu_2O-based catalysts for electrochemical CO_2 reduction via *in-situ* ATR-IR and Raman. **Z. Liang**, J. Fu, M.B. Vukmirovic, R.R. Adzic

Section E
Hampton Inn & Suites Convention Center
Fulton

R&D in the Chemical Catalysis for Bioenergy Consortium

Cosponsored by ENFL, ENVR and INOR
S. Habas, D.A. Ruddy, *Organizers*
J. Schaidle, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CATL 282. ChemCatBio: Overview of the US Department of Energy's chemical catalysis for bioenergy consortium. **N.D. Fitzgerald**, G.J. Leong

1:25 CATL 283. Activation of isobutane over a Cu/BEA catalyst and re-incorporation into the chain growth cycle of DME homologation. **D.A. Ruddy**, C. Nash, C. Farberow, J. Hensley, J. Schaidle

1:45 CATL 284. Renewable and recycled carbon for high octane low carbon gasoline (HOLCG) production at pilot scale. **S.C. Marie-Rose**, D. Ruddy, J. Hensley

2:05 CATL 285. Accelerating the development of catalysts for biofuel production through the application of x-ray absorption spectroscopy. **T. Krause**, C. Yang, A.J. Kropf, J. Miller, D. Ruddy, J. Schaidle, S. Cheah, K.A. Unocic, S. Habas

2:25 Intermission.

2:40 CATL 286. Catalytic conversion of fermentation derived ethanol to advanced hydrocarbon fuels and valuable chemicals. **Z. Li**, A. Lepore, M. Salazar, B.H. Davison, C.K. Narula

3:00 CATL 287. Advanced characterizations to accelerate commercial catalyst development for ethanol upgrading technology. **J. Hannon**

3:20 CATL 288. MgO-Al_2O_3 supported copper pseudo single atom catalysts for Guerbet ethanol conversion. **K.K. Ramasamy**, M. Guo, M. Gray, S. Subramaniam

3:40 CATL 289. Mixed metal oxide (MMO) catalysts for single step conversion of bio-based C2-C6 oxygenates to olefins processes. **J.O. Smith**

4:00 CATL 290. Single-step conversion of ethanol to butadiene over Ag-ZrO_2/SiO_2 catalysts. V. Lebarbier Dagle, **R. Dagle**, J. Saavedra Lopez, M. Flake, T. Lemmon

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Enabling Fundamental Advances in Catalysis & Surface Science

Cosponsored by ENVR, INOR and PHYS
W.O. Gordon, *Organizer*
M.L. McEntee, J. Pietron, *Organizers, Presiding*
W. Gordon, *Presiding*

1:00 CATL 291. Fundamental concepts in catalyst design. **C.T. Campbell**

1:30 CATL 292. Operando investigation on the structure and reactivity of adsorbed NH_3, NOX & V=O species during SCR on shaped vanadia catalyst. M.A. Banares, **S.B. Rasmussen**, R. Portela, P. Bazin, H. Falsig, A. Godiksen, P. Georg Moses, M. Daturi

1:50 CATL 293. Insights into the deactivation of Cu/SAPO-34 by low- and high-temperature hydrothermal treatment. **F. Gao**, A. Wang, E.D. Walter, Y. Zheng, J. Szanyi, Y. Wang, C.H. Peden

2:10 CATL 294. Organic ligand promotion effect on CeO_2-catalyzed NH_3-SCR. **L. Chen**, V. Agrawal, S.L. Tait

2:30 CATL 295. Multi-component homogeneous and heterogeneous catalysts involving Br_x/NO_x systems for selective aerobic decontamination. **K. Sullivan**, Y.V. Geletii, M. Kim, D. Collins-Wildman, Q. Yin, C.L. Hill

2:50 Intermission.

3:05 CATL 296. Ultrahigh vacuum surface science investigations of chemical warfare agent chemistry within Zr (IV) MOFs. C.H. Sharp, T. Grissom, D. Troya, A. Plonka, A.J. Morris, P. Usov, W.O. Gordon, **J.R. Morris**

3:35 CATL 297. Chemical warfare agent decontamination on zirconium hydroxide under *operando* conditions. **P. Pehrsson**, R. Balow, D. Barlow, M.L. McEntee, W.O. Gordon, J. Lundin, G.C. Daniels, S.L. Giles, M. Hall, J.H. Wynne, G.W. Peterson

4:00 CATL 298. In situ studies of Zr-based MOFs for nerve-agents capture and decomposition. **A. Plonka**, Q. Wang, W.O. Gordon, A. Balboa, D. Troya, W. Guo, C.H. Sharp, S.D. Senanayake, J.R. Morris, C.L. Hill, A.

‡*Cooperative Cosponsorship*

Frenkel

4:20 CATL 299. Impact of ambient gases on the mechanism of the $[Cs_8Nb_6O_{19}]$-catalyzed nerve-agent decontamination. **J. Musaev**, A. Kaledin, D. Driscoll, D. Troya, D. Collins-Wildman, C.L. Hill, J.R. Morris

4:40 CATL 300. Multifaceted role of buffer anions in polyoxometalate-catalyzed organophosphorus ester hydrolysis. **D.L. Collins-Wildman**, M. Kim, K. Sullivan, J. Musaev, C.L. Hill

Computational Catalyst Design for Energy Conversion & Storage

Development of Homogeneous & Heterogeneous Catalysts

Sponsored by COMP, Cosponsored by CATL and CINF

ACS Award Lectures
Sponsored by COLL, Cosponsored by CATL‡

Carbon Dioxide Conversion & Artificial Photosynthesis

Electro-Photo Catalytical Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

General Catalysis

A. Savara, *Organizer*

7:00–9:00

CATL 301. Fabrication of porous MnO_x-FeO_x nanoneedles for the selective catalytic reduction of NO_x by NH_3 at low temperature. **Z. Fan**, **J. Shi**, C. Niu

CATL 302. Preparation and characterization of a Ni on carbon fixed bed catalyst and evaluation of its efficiency as a catalyst in hydrogenation of furfural. **R. Adhikari**, T.V. Kotbagi, M.G. Bakker

CATL 303. Synthesis and characterization of Cu loaded on mesoporous CeO_2-TiO_2. **D. Ongmali**, T. Chaisuwan, A. Luengnaruemitchai, S. Wongkasemjit

CATL 304. Pd–Pt alloy on Fe_3O_4 for tandem ammonia borane dehydrogenation/nitroarene reduction as magnetically recyclable nanoatalysts. **S. Byun**, B. Kim

CATL 305. Development of a AuPd alloy on Fe_3O_4 for one-pot cascade nitro-reduction and reductive amination, and efficient isoindolinone synthesis. **A. Cho**, B. Kim

CATL 306. Selective catalytic oxidation of ammonia in air at ambient temperature: Evidence of direct $N_2H_6^+$ route. H. Chen, **M. Arjona Alonso**, W. Han, K. Yeung

CATL 307. Controlling product selectivity for electrochemical reduction of CO_2 on gold by pulsing potentials. **J.J. Fuentes-Rivera**, K. Kimura, T. Hanrath

CATL 308. Catalyst-controlled stereoselective *O*-glycosylation: Pd(0) vs Pd(II). **H. Yao**, S. Zhang, W. Leng, M. Leow, S. Xiang, J. He, H. Liao, K. Le Mai Hoang, X. Liu

CATL 309. Catalytic removal of Hg^{2+} in Hg contaminated agricultural water by ionic liquids: A density functional theory study. X. Song, P. Ning, C. Wang, **K. Li**, **M. Fan**

CATL 310. Density functional theory study on catalytic synthesis of NH_3 from N_2 and H_2O over FeO. X. Song, P. Ning, C. Wang, **K. Li**, **M. Fan**

CATL 311. Bi metal modified $Bi_4O_5I_2$ hierarchical microsphere with oxygen vacancies for the improved photocatalytic performance and mechanism insights. **X. Liu**, **D. Shuoping**, **J. Hu**

CATL 312. In-situ topotactic synthesis and photocatalytic activity of plate-Like biOCl/2D networks Bi_2S_3 heterostructures. **Y. Shi**, X. Liu, D. Shuoping, J. Hu

CATL 313. Synthesis and characterization of single-crystalline $Bi_{19}Cl_3S_{27}$ nanorods. **W. Zuozuo**, Z. Huang, J. Hu

CATL 314. Synthesis and characterization of single-crystalline $Bi_2O_2SiO_3$ nanosheets with exposed {001} facets. **D. Shuoping**, X. Liu, J. Hu

CATL 315. Decontamination of HD and its simulant on BODIPY-doped polymer films by photooxidation under visible light. **H. Wang**, G.W. Wagner, A.X. Lu, C.J. Karwacki

CATL 316. A novel method for preparing highly dispersed Ni_2P/functionalized CMK-3 catalysts for the hydrodesulfurization of 4,6-DMDBT. **T. Huang**, J. Xu, F. Yu

CATL 317. Influence of Fe site location in Fe-MFI zeolite catalysts on the performance of hydroxylation of benzene to phenol with H_2O_2. **P. Xiao**, J.N. Kondo, T. Yokoi

CATL 318. Fe-NbP as an effective catalyst for levulinic acid production from glucose: Characterization and performance. **W. Wei**, H. Yang, X. Liu, S. Wu

CATL 319. Identifying the non-stoichiometric ZnCr2O4 with excess Zn as the active high-temperature methanol synthesis catalyst. H. Song, J. Carey, **M. Nolan**, M. Muhler

CATL 320. Mild base-catalyzed dehydrosilylation of alcohols with hydrosilanes. **N.A. DeLucia**, A.K. Vannucci

CATL 321. Nickel dual photoredox catalysis for the synthesis of aryl amines. **R. Key**, A.K. Vannucci

CATL 322. Operando reaction study of toluene oxidation over ceria catalysts. Q. Wang, **M. Arjona Alonso**, M.A. Bañares, K. Yeung

CATL 323. Biosynthesized palladium nanoparticles mediated by black pepper extract as highly efficient and reusable nanocatalyst in aryl halide cyanation and Hiyama cross-coupling reactions under ligand free conditions. V. Kandathil, S. Patil, **S. Patil**

CATL 324. Investigation of Pd/CeO_2 catalysts for acetylene selective hydrogenation. **T. Lyu**

CATL 325. Conversion of isobutanol into olefins and aromatics: Product distribution control and reaction mechanism study. B. Zhang, **Z. Du**, W. Li

CATL 326. One pot synthesis of ordered mesoporous Ni-SiO_2-Al_2O_3 for hydrodeoxygenation of dibenzofuran as coal tar model compound. H. Peng, **Z. Du**, W. Li

CATL 327. Whole-cell biocatalyst-mediated acylation of vitamin P-like bioflavonoids in binary organic solvents. X. Xin, **X. Li**, **G. Zhao**

CATL 328. Highly efficient biocatalysis for the acylation of flavonoids and dimethyl azelate. H. Xu, **X. Li**, **G. Zhao**

CATL 329. Synthesis and characterization of Ti-MWW zeolite with different Ti atom distributions. **X. Ji**, J.N. Kondo, T. Yokoi

CATL 330. Development of novel Pd-ceria catalyst system for selective hydrogenation of acetylen. **S. Kim**, W. Jang

CATL 331. Photoactive palladium (II) complexes for Sonogashira reactions. **K. Dissanayake**, H. He

CATL 332. Synthesis of high surface area mesoporous catalysts from carbon sources for the production of biodiesel. **M. Omer**, W. Jang

CATL 333. Alumina supported monometallic and bimetallic palladium catalysts for liquid phase semi-hydrogenation of alkynes. **S. Hussaini**, W. Jang, B. Ni, K. Mackenzie

CATL 334. Hydrocracking of kraft and biorefinery lignins using a dual acid-base catalyst. **M. Kollman**, H. Jameel, H. Chang, W. Li

CATL 335. Gemini surfactant-assisted synthesis of Mo-based precursors for preparing NiMo/SiO_2-Al_2O_3 hydrodesulfurization catalysts. **J. Xu**, T. Huang, F. Yu

CATL 336. Copper-gold nanoparticles encapsulated within surface-tethered dendrons as supported catalysts for the click reaction. **A. Koishybay**, D.F. Shantz

CATL 337. Synthesis of SAPO-11 molecular sieve in ethylene glycol and supercritical carbon dioxide. **C. Wen**, **F. Yu**

CATL 338. Withdrawn

CATL 339. Study on acylation of puerarin catalyzed by whole cells in non-aqueous medium. T. Yuan, **X. Li**, **G. Zhao**

CATL 340. Plasma synthesis, characterization and catalytic activity of mixed oxide ferrites. **N. Dumaresq**, A.H. Moores, N. Braidy

CATL 341. Guerbet reaction of ethanol over Cu doped porous metal oxides: Effects of chloride poisoning. **J.A. Barrett**, Z. Jones, C. Stickelmaier, N. Schopp, P.C. Ford

CATL 342. Ceria loading and pretreatment effects on Pd/Al_2O_3 for selective hydrogenation of acetylene. **A. Bradicich**, W. Jang

CATL 343. Hollow structure of ZSM-5 aggregate prepared by desilication with surfactants: A superior MTP catalyst. **Y. Song**, Y. Shang, Z. Zhao, X. Zhao, T. Ma, J. Wei, Y. Gong

CATL 344. Mechanism of the acetonitrile hydrogenation to amines over a platinum catalyst investigated by in situ infrared spectroscopy and DFT modeling. L. Vogt, P. Quaino, **F.C. Calaza**, S. Collins

CATL 345. Electrochemical reduction of carbon dioxide over bimetallic metal-on-copper electrocatalysts. **Y.F. Nishimura**, C. Hahn, T.F. Jaramillo

CATL 346. Alcohol assisted methane dehydroaromatization over different Mo_2C- containing zeolite catalysts. **R. Thakur**, R. Adams, C.A. Carrero

CATL 347. Improving hydrogen production from ammonia borane hydrolysis by using acid supports. R. Gil-San Millán, A. Grau-Atienza, N. Linares, **J. Garcia Martinez**

CATL 348. Immobilization of enzymes onto 2D and 3D supports and characterization using surface science techniques. **T. Hurlburt**, M.B. Francis, G.A. Somorjai

CATL 349. Surface roughness effects on catalytic performance of metal oxides over-layers on SBA-15. **T. Lozano**, M.A. Smith

CATL 350. Stereolithographic 3D printing of catalytic devices from bifunctional molecular precursors. **J. Manzano**, Z.B. Weinstein, A.D. Sadow, I.I. Slowing

CATL 351. Predicting formate selectivity from CO2 using bimetallic alloys. **M. Inouye**, M. Groves

CATL 352. A universal strategy for visible-light-driven H_2 production integrated with biomass upgrading. **G. Han**, Y. Sun

CATL 353. A palladium based catalyst in the selective oxidation of cyclohexane by aqueous hydrogen peroxide. **C. Zhang**, Q. Zhao

CATL 354. Synthesis and catalytic activity of $NiMoS_2$ in the removal of dibenzothiophene from model fuels. **J.R. Luna**, H.M. Morales, J. Parsons

WEDNESDAY MORNING

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Kinetics

Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

8:00 CATL 355. Reaction kinetics analysis of Pd-catalyzed C-Cl hydrogenolysis in aromatic systems. M. Al-Gharrawi, M.C. Wheeler, **T.J. Schwartz**

‡*Cooperative Cosponsorship*

8:20 CATL 356. Acid site proximity effects on methanol dehydration catalysis by zeolites. J.R. Di Iorio, C.T. Nimlos, S. Nystrom, A. Hoffman, D. Hibbitts, **R. Gounder**

9:00 CATL 357. Mechanistic insight into the exceptional activity and selectivity of bimetallic Pd-Cu alloy catalysts for alcohol dehydrogenation. Y. Song, K. Goulas, D. Toste, **L. Grabow**

9:20 CATL 358. Mechanistic investigation of the deoxydehydration of sugar alcohols over ReOx-Pd/CeO2 catalysts. Y. Xi, **A. Heyden**

9:40 Intermission.

10:00 CATL 359. Molecular-level insights into how the structure of liquid water influences the mechanism of sugar alcohol decomposition in aqueous phase heterogeneous catalysis. C.J. Bodenschatz, T. Xie, **R.B. Getman**

10:20 CATL 360. Catalysis for upgrading C_1 feedstocks. **A. Bhan**

11:00 CATL 361. Stabilization of transition states by solvation: Inorganic hosts, liquids, and dense adlayers. **E. Iglesia**

11:40 CATL 362. Mechanism and kinetics of selective acylation reactions with carboxylic acids over Brønsted acid sites. A. Gumidyala, I. Alalq, B. Wang, **S. Crossley**

Section B
Hampton Inn & Suites Convention Center
Riverside I

New Techniques & Applications of Magnetic Resonance Methods in Heterogeneous Catalysis

F.A. Perras, N. Washton, *Organizers*
S.L. Scott, *Organizer, Presiding*

8:00 CATL 363. Direct observation of three-dimensional atomic-level structures on the surface of catalytic nanoparticles. **L. Emsley**

8:40 CATL 364. Combining surface organometallic chemistry and advanced solid-state NMR techniques (SENS-DNP) allows yielding and understanding molecular single site catalysts. **C. Thieuleux**

9:00 CATL 365. Obtaining quantitative structural parameters in amorphous heterogeneous catalysts using advanced DNP-enabled recoupling approaches. **F.A. Perras**, T. Kobayashi, M. Pruski

9:20 CATL 366. DNP NMR of adsorption and exchange at a silicon surface. M. Guy, K.J. van Schooten, L. Zhu, **C. Ramanathan**

9:40 Intermission.

10:00 CATL 367. NMR methods applied to quadrupolar nuclei for the structural study of supported catalysts. **L. Delevoye**, N. Merle, I. Del Rosal, L. Maron, M. Taoufik, R. Gauvin

10:40 CATL 368. Probing ionic liquid electrolyte structuring in the glassy state by DNP NMR spectroscopy. P. Martin, M. Sani, R. Yunis, F. Chen, M. Deschamps, M. Forsyth, **L. O'Dell**

11:00 CATL 369. Compositions and structures of high-N-content mesoporous carbon electrocatalysts analyzed by solid-state NMR. **B. Chmelka**, N.P. Zussblatt, N. Fechler, M. Antonietti

Section C
Hampton Inn & Suites Convention Center
Riverside III

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Cosponsored by ENFL, ENVR and INOR
J. Choi, O. Gazit, M. Kidder, *Organizers, Presiding*

8:00 CATL 370. Selective aerobic oxidation of bio-derived molecules over nanostructured catalysts. **A.F. Lee**

8:30 CATL 371. Cost-effective synthesis of 1, 3-cyclopentanediol with furfuryl alcohol derived from lignocellulose. **G. Li**, N. Li, A. Wang, T. Zhang

8:45 CATL 372. Catalytic conversion of bioderived muconic acid to produce drop-in cyclic monomers and functional alternatives. **A. Settle**, L. Berstis, N. Rorrer, H. Hu, R.M. Richards, G. Beckham, M.F. Crowley, D. Vardon

9:00 CATL 373. Directed Glycerol reforming through tailored platinum nanoparticles. **J. Callison**, S. Rogers, N.D. Subramanian, D. Gianolio, R. Catlow, P. Wells, N. Dimitratos

9:15 CATL 374. Conversion of model, waste and highly unsaturated lipids to fuel-like hydrocarbons over bimetallic decarboxylation/decarbonylation catalysts. **E. Santillan-Jimenez**, R. Loe, Y. Song, M. Isaacs, A. Lee, K. Wilson, M. Crocker

9:45 Intermission.

10:00 CATL 375. Regioselectivity and chemoselectivity in heterogeneously catalyzed cross-aldol condensations with unsymmetrical ketones. K. Ponnuru, J.C. Manayil, H. Cho, A. Osatiashtiani, W. Fan, K. Wilson, **F. Jentoft**

10:30 CATL 376. Controlled deoxygenation of citric and amino acids towards valuable chemicals. **J. Verduyckt**, R. Coeck, A. Geers, M. Van Hoof, D. De Vos

10:45 CATL 377. Catalytic multistage process for the production of polyhydroxyalkanoate monomers from bioethanol. M. Ruiz-Ramiro, D. Santhanaraj, M. Komarneni, T. Pham, D.E. Resasco, **J. Faria**

11:00 CATL 378. Synthesis of high-molecular-weight polycarbonates from bio-based isosorbide catalyzed by metal-free ionic liquids. **C. Ma**, W. Cheng, F. Xu, S. Zhang

11:15 CATL 379. Catalytic hot gas filtration for tailoring vapor chemistry of fast pyrolysis bio-oils. **M. Lu**, M.Z. Hu, J. Choi

11:30 CATL 380. Development of hydrothermally stable materials for the catalytic upgrading of biomass-derived carboxylic acids in the presence of condensed water. J. Lopez-Ruiz, A. Cooper, G. Li, T. Varga, M. Engelhard, L. Kovarik, **K.O. Albrecht**

Section D
Hampton Inn & Suites Convention Center
Bienville

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Cosponsored by COMP and ENFL
A. Savara, *Organizer*
V.G. Baldovino-Medrano, J.J. Bravo-Suarez, *Organizers, Presiding*

8:00 CATL 381. Control over and Impact of the silver particle size in Ag/β-alumina epoxidation catalysts. **P. de Jongh**, J. van den Reijen, K. De Jong

8:40 CATL 382. Ethylene oxidation by promoted supported Ag/Al_2O_3 catalysts: A fundamental perspective of an industrial catalyst. **I.E. Wachs**, J. Jehng, M.E. Ford

9:05 CATL 383. Effect of catalyst crystallinity on deactivation for olefin epoxidation utilizing organic hydroperoxide as oxidant. **A.S. Katz**, M. Aigner, C. Schoettle, A. Okrut, S.I. Zones, N.G. Grosso-Giordano

9:30 CATL 384. Transitioning rationally designed catalytic materials to real ''working'' catalysts produced at commercial scale: Nanoparticle materials. **J. Hensley**, S. Habas, F. Baddour, C. Farberow, D. Ruddy, J. Schaidle, R.L. Brutchey, N. Malmstadt, H.J. Robota

9:55 Intermission.

10:15 CATL 385. Multiscale modeling of the electrochemical reduction of CO_2. **A.T. Bell**

10:40 CATL 386. Extrusion of β-MnO2 catalysts for styrene combustion. **V.G. Baldovino-Medrano**, M. Savastano, B. Kartheuser, E.M. Gaigneaux

11:05 CATL 387. Industrial preparation of unsymmetrical ketones through the lens of academic exercises on the catalytic decarboxylative ketonization mechanism. **A. Ignatchenko**

11:30 CATL 388. Activation of TiO_2 by anchoring transition metal cations for partial oxidation of methane. **F. Tao**

Section E
Hampton Inn & Suites Convention Center
Fulton

R&D in the Chemical Catalysis for Bioenergy Consortium
Cosponsored by ENFL, ENVR and INOR
S. Habas, J. Schaidle, *Organizers*
D.A. Ruddy, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CATL 389. Dual single-atom sites for hydordeoxygenation of bio-oil molecules to hydrocarbons. **F. Tao**

8:25 CATL 390. *Ex situ* catalytic fast pyrolysis over Pt/TiO_2: Fixed bed hydrodeoxygenation followed by hydrotreating to produce fuel blendstocks. **M. Griffin**, C. Mukarakate, K. Iisa, K. Orton, R.J. French, K.A. Magrini, M. Jarvis, J. Olstad, H. Wang, A. Dutta, F.G. Baddour, K.M. Van Allsburg, G. Ferguson, D.A. Ruddy, G. Beckham, J. Schaidle

8:45 CATL 391. Catalytic fast pyrolysis of biomass using Mo_2C unravels promise and challenges with HDO catalysts. **C. Mukarakate**, K. Iisa, K. McKinney, M. Xu, R.J. French, C. Nash, M. Griffin, S. Habas, M.R. Nimlos, D. Ruddy, J. Schaidle

9:05 CATL 392. Durability of molybdenum carbide catalysts in reductive upgrading of fast pyrolysis bio-oil. **J. Choi**, K.A. Unocic, Z. Wu, H. Wang, A.H. Zacher, S. Habas

9:25 CATL 393. *In situ* S/TEM closed-cell gas reactions of catalysts: Capabilities and opportunities. **K.A. Unocic**, J. Choi, D. Ruddy, J. Schaidle, T. Krause, C. Mukarakate, M. Xu, S. Habas

9:45 Intermission.

10:00 CATL 394. Advances in nanoscale metal carbide and phosphide catalysts for biomass conversion processes. **S. Habas**, F. Baddour, D. Ruddy, J. Schaidle

10:20 CATL 395. Continuous flow synthesis of nanoparticle catalysts as a safe and sustainable nanomanufacturing method. **R.L. Brutchey**

10:40 CATL 396. Catalyst cost estimation tool development: Reducing information barriers to commercialization. K. Van Allsburg, J.D. Super, J.F. White, J. Schaidle, L. Snowden-Swan, **F. Baddour**

11:00 CATL 397. Multifunctional metal-organic framework catalysts for hydrogen activation. **M. Allendorf**, M. Foster, V. Stavila

11:20 CATL 398. Tandem and aqueous phase heterogeneous catalytic systems. **B.G. Trewyn**, M. Moyer

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Catalysis & Surface Science Science Applied to the Destruction of Threat Agents

Cosponsored by ENVR, INOR and PHYS
W.O. Gordon, *Organizer*
M.L. McEntee, J. Pietron, *Organizers, Presiding*
W. Gordon, *Presiding*

8:00 CATL 399. Bioengineering and nanoscience solutions for chemical and biological defense. **R. Botto**

8:30 CATL 400. Oxidation-stable plasmonic copper nanoparticles in catalytic TiO_2 aerogels. **P. DeSario**, J. Pietron, T.H. Brintlinger, J.F. Parker, O.A. Baturina, R. Stroud, D.R. Rolison

8:55 CATL 401. Plasmonic $Ag\text{-}TiO_2/TiO_x$ nanocomposites for enhanced visible light photocatalysis of chemical threats. **D.L. Kuhn**, B.G. DeLacy, Z. Zander

9:20 CATL 402. A combined theoretical and experimental investigation on the degradation of organophosphorus chemical warfare agents on ZnO_{1-x}. **J. Landers**, N. Zougheib, F.E. Celik, A.V. Neimark

9:40 CATL 403. First-principles calculations of nerve agent adsorption on anatase surfaces. **N.Q. Le**, C. Ekuma, B.I. Dunlap, D. Gunlycke

10:00 Intermission.

10:15 CATL 404. Materials for decontamination of chemical agents:

‡*Cooperative Cosponsorship*

Multimodal investigation of active sites. **A. Frenkel**, Y. Tian, A.M. Plonka, D. Troya, C.H. Sharp, J.R. Morris, J. Musaev, S.D. Senanayake, D.L. Collins-Wildman, C.L. Hill, M.B. Mitchell, W.O. Gordon

10:45 CATL 405. Protection by simultaneous toxic-agent-induced barrier formation and catalytic decontamination. **C.L. Hill**, K. Sullivan, D. Collins-Wildman, Q. Yin, E.R. Weeks, T. Liu

11:15 CATL 406. Efficient MOF-based degradation of organophosphates in non-aqueous environments. **D.F. Sava Gallis**, J. Harvey, C.J. Pearce, J. DeCoste, M.K. Kinnan, J.A. Greathouse

11:35 CATL 407. Exploring catalytic hydrolysis of organophosphorus nerve agents and their simulants by the metal-organic framework NU-1000. **M. Mendonca**, H. Chen, P. Liao, R. Snurr

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

WEDNESDAY AFTERNOON

Section A
Hampton Inn & Suites Convention Center
Antonine

Unconventional Catalysis Targeting Stable Molecules
Cosponsored by ENFL, ENVR, INOR and PHYS
C. Wang, *Organizer*
C.L. Marshall, *Organizer, Presiding*
C. Wang, *Presiding*

1:00 CATL 408. Catalytic H/D exchange with supported Ir(III) complexes as a probe reaction for metal–support interactions. D. Kaphan, R. Klet, **M. Delferro**

1:20 CATL 409. Unconventional oxide/metal catalysts for CO_2 activation and conversion. **J. Rodriguez**

2:00 CATL 410. Delineating heavy oil deviscosification catalytic chemistry of metal sulfonates. Y. Xi, C. Ayala Orozco, **M.S. Wong**

2:40 Intermission.

2:50 CATL 411. Diamonds from the sky: Facile, inexpensive transformation of the greenhouse gas carbon dioxide into carbon nanotube wool. **S.L. Licht**

3:30 CATL 412. The role of hydrides in ammonia synthesis. J. Guo, P. Wang, F. Chang, W. Gao, **P. Chen**

Section B
Hampton Inn & Suites Convention Center
Riverside I

New Techniques & Applications of Magnetic Resonance Methods in Heterogeneous Catalysis

S.L. Scott, N. Washton, *Organizers*
F.A. Perras, *Organizer, Presiding*

1:00 CATL 413. Solid-state NMR investigation of alumina and of alumina-supported organometallic catalysts. N. Merle, F. Pourpoint, K.C. Szeto, F. Zhang, S.L. Scott, M. Taoufik, L. Delevoye, **R. Gauvin**

1:40 CATL 414. Demystifying atomic environments within heteroatom substituted zeolite frameworks with solid-state nuclear magnetic resonance. **V.K. Michaelis**, M. Ha, J. Lewis, H. Luo, W. Gunther, Y. Roman-Leshkov

2:00 CATL 415. Developing an understanding of the oligomerization of light olefins over MTW zeolite based catalysts using NMR. **C.P. Nicholas**, S. Prabhakar

2:20 CATL 416. Operando EPR in heterogeneous catalysis – Step child or bright spot? **A. Brueckner**

3:00 Intermission.

3:20 CATL 417. New insights into the activity of heterogeneous catalysts by probing proximities between ^{1}H and quadrupolar nuclei using high-field NMR. J. Trébosc, W. Qiang, J. Xu, F. Pourpoint, J. Huang, F. Deng, J. Amoureux, **O. Lafon**

4:00 CATL 418. Internal field ^{59}Co NMR study of cobalt-iron nanoparticles during the activation of $CoFe_2/CaO$ catalyst for carbon nanotube synthesis. A.S. Andreev, D.V. Krasnikov, M. Kazakova, O.B. Lapina, V.L. Kusnetsov, **J. d'Espinose de Lacaillerie**

4:20 CATL 419. Relationships between molecular structure & chemical bonding and quadrupolar & nuclear magnetic shielding tensors in catalytically active systems and model compounds. **J. Autschbach**, M. Srebro-Hooper, E. Zurek

Section C
Hampton Inn & Suites Convention Center
Riverside III

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Cosponsored by ENFL, ENVR and INOR
J. Choi, O. Gazit, M. Kidder, *Organizers, Presiding*

1:00 CATL 420. Cleavage of C-C bond: A key step in the biomass conversion to chemicals. **A. Wang**

1:30 CATL 421. Withdrawn

1:45 CATL 422. Carboxylic acid conversion over doped molybenum carbides. **A. Lepore**, Z. Li, J. Choi

2:00 CATL 423. Effect of physicochemical properties of $Ce_{1-x}Zr_xO_2$ solid solutions on carbonylation of glycerol with CO_2 into glycerol carbonate. **L. Jiaxiong**, D. He

2:15 CATL 424. Waste water to chemicals via bioelectrochemically derived hydrogen peroxide and tandem catalysis. E. Taw, J. Griffin, A.A. Gosavi, K.A. Gray, **J.M. Notestein**, G. Wells

2:45 Intermission.

3:00 CATL 425. Ketonization of volatile fatty acids recovered from waste water streams. E. Fufachev, B. Weckhuysen, **P. Bruijnincx**

3:30 CATL 426. Hydrodeoxygenation of stearic acid over $NiMo/\beta\text{-}Al_2O_3$ catalyst. **P. Kumar**, S.K. Maity, D. Shee

3:45 CATL 427. Indirect oxidation of glucose to glucuronic acid using Pd-decorated Au catalysts. **Y. Yin**, L. Chen, Z. Zhang, M.S. Wong

4:00 CATL 428. Effect of noble and non-noble metals on the electrocatalytic reduction of whole pyrolysis oil. **J. Egbert**, R. Weber, J. Holladay

4:15 CATL 429. Electrocatalytic and photocatalytic conversion of biomass derived molecules coupled with hydrogen production. **Y. Sun**

4:30 CATL 430. Ring rearrangement reactions of furanic species over metals supported on reducible oxides. **S. Crossley**, L. Herrera, A. Gomez

5:00 Concluding Remarks.

Section D
Hampton Inn & Suites Convention Center
Bienville

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Cosponsored by COMP and ENFL
A. Savara, *Organizer*
V.G. Baldovino-Medrano, J.J. Bravo-Suarez, *Organizers, Presiding*

1:00 CATL 431. Simple, effective nanoparticle synthesis via electrostatic adsorption using incipient wetness impregnation. S. Eskandari, G. Tate, **J.R. Regalbuto**

1:40 CATL 432. Bifunctional catalyst: From macroscopic to molecular understanding. **E. Gutierrez Acebo**, C. Bouchy, C. Chizallet, Y. Schuurman

2:05 CATL 433. Modeling of catalytic reactors for light alkane dehydrogenation. **X. Nijhuis**, A. VandePutte

2:30 CATL 434. DME to alkylate: Implications of catalyst performance on commercialization. **J. Hensley**, C. Nash, C.A. Farberow, D. Ruddy, J. Schaidle

2:55 Intermission.

3:15 CATL 435. Molecular level understanding of heterogeneous catalysts for olefin polymerization. **S.L. Scott**

3:40 CATL 436. Carbon nanotube-supported catalysts prepared by a modified photo-Fenton process for Fischer-Tropsch synthesis. H. Almkhelfe, X. Li, K.L. Hohn, **P.B. Amama**

4:05 CATL 437. Technical catalyst development for conversion of biogas to liquid fuels. X. Zhao, D. Walker, T. Roberge, P. Stachurski, M. Kastelic, S. Shah, B. Joseph, **J. Kuhn**

4:30 CATL 438. Multiscale modeling "from electrons to reactors": CO oxidation over RuO2. J.E. Sutton, J. Lorenzi, S. Matera, **A. Savara**

4:55 CATL 439. Multi-scale modelling, synthesis and characterization of materials for chemical looping reforming. **S. Andersson**, P. Dahl, S. Radl, I. Svenum, S. Cloete, S. Shevlin, A. Zaabout, J.R. Tolchard, Z. Guo, S. Amini

5:20 CATL 440. Development and scale-up of structured catalytic reactors for steam methane reforming. **J. De Wilde**

Section E
Hampton Inn & Suites Convention Center
Fulton

R&D in the Chemical Catalysis for Bioenergy Consortium
Cosponsored by ENFL, ENVR and INOR
D.A. Ruddy, J. Schaidle, *Organizers*
S. Habas, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CATL 441. Deactivation of zeolite catalysts during hydrodeoxygenation of aromatic oxygenates. C. Okolie, M. Veiga Rodrigues, G. Foo, M. Yung, **C. Sievers**

1:25 CATL 442. Study of residence time distribution in a circulating fluidized bed reactor for biomass pyrolysis vapor upgrading. X. Gao, T. Li, **W. Rogers**

1:45 CATL 443. Measurement and simulation of coking of catalyst particles in vapor phase upgrading. **J. Parks**, P. Ciesielski, K. Unocic, M. Pecha, V.S. Bharadwaj, D. Robichaud, B. Kappes

2:05 CATL 444. Upgrading of direct liquefaction aqueous waste stream: Experimental and economic assessment. S. Davidson, J. Lopez-Ruiz, A. Cooper, Y. Zhu, R. Dagle, **K.O. Albrecht**

2:25 Intermission.

2:40 CATL 445. Catalytic upgrading of biochemically derived intermediates from lignocellulosic biomass to advanced biofuels and chemicals. **R. Elander**, D.K. Johnson, D. Vardon, Z. Li, C.K. Narula, B.H. Davison, A.D. Sutton, A.B. Padmaperuma, M. Lilga

3:00 CATL 446. Simultaneously producing fuels and chemcials from bioderived molecular building blocks. **A.D. Sutton**, C. Moore, R. Jenkins, T. Semelsberger, O. Staples, W. Kubic

3:20 CATL 447. Selective electrochemical reduction of CO_2 to high-value chemical precursors for integration with biological processes. **E. Cave**, K. Kuhl, S. Ma, G. Leonard, N. Flanders

3:40 CATL 448. Catalytic coupling of short chain microbial acids to biofuel precursors. **D. Vardon**, A. Settle, N. Cleveland, J. Stunkel

4:00 CATL 449. Understanding catalyst activity and durability through computational methods: The case of RuSn. **D. Robichaud**, V. Vorotnikov, S. Kim, G. Beckham, L.A. Curtiss, R. Assary

Section F
Hampton Inn & Suites Convention Center
Cottonmill

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Photocatalytic Approaches

Cosponsored by ENVR, INOR and PHYS
W.O. Gordon, *Organizer*
M.L. McEntee, J. Pietron, *Organizers, Presiding*
W. Gordon, *Presiding*

1:00 CATL 450. Correlation of the chemistry of chemical warfare agents with that of simulants on advanced materials using in situ & operando methods. **W.O. Gordon**, M.L. McEntee, A. Balboa, G.W. Peterson, A. Frenkel, J. Pietron, J.R. Morris, S.D. Senanayake, M.B. Mitchell, P. Pehrsson

‡*Cooperative Cosponsorship*

1:30 CATL 451. Photocatalytic oxidation of water soluble organic and pharmaceutical compounds using visible/near uv light. **R.D. Barreto**, M. Howell

1:50 CATL 452. Investigation of a facile, scalable synthesis route for bismuth oxychloride 2D nanostructures for photocatalytic water treatment. M. Robinson, S. Padilla, A. Pattammattel, L. Gómez-Velázquez, M. Bizarro Sordo, **V. Leppert**

2:10 CATL 453. Synthesis and application of a sustainable N-doped TiO_2/CdS nanohybrid composite for photocatalytic degradation of 4-chlorophenol. **A. Aragon**, W. Kierulf-Vieira, T. Lecki, M. Skompska, J. Widera

2:30 Intermission.

2:45 CATL 454. Solar-light driven photocatalytic degradation of organic pollutants using natural dye-sensitized TiO_2. **M. Ghosh**, A. Ray

3:05 CATL 455. Improvement of photoelectrochemical activity of ZnO/TiO2 core-shell nanostructure through Ag nanoparticle integration. **Z. Wang**, X. Wang

3:25 CATL 456. Oxygen-doped nanoporous carbon nitride via water-based homogeneous supramolecular assembly for photocatalytic hydrogen evolution. **Z. Jingwen**, J. Zou, L. Pan

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

THURSDAY MORNING

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces
Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

9:00 CATL 457. Kinetic consequences of carbon and oxygen coverages during CO_x methanation and CH_4 dry reforming on Ni, Co, and Ni-Co clusters. **P.T. Lachkov**, Y. Chin

9:20 CATL 458. Investigating alkene formation pathways in methanol-to-hydrocarbon processes within zeolites. **P. Kravchenko**, M. Deluca, D. Hibbitts

9:40 CATL 459. On the role of surface adsorbed oxygen in ethanol reaction pathways on Mo_2C. **C.A. Farberow**, C. Nash, J. Hall, J. Schaidle

10:00 CATL 460. Nature of the active sites for carbon dioxide reduction on metal nanoparticles: suggestions for optimizing performance. **T. Cheng**, Z. Wang, W.A. Goddard

10:20 Intermission.

10:40 CATL 461. Understanding activity loss in precious-metal combustion catalysts using well-defined nanocrystals. **E.D. Goodman**, A. Riscoe, N. Tahsini, F. Abild-Pedersen, A.C. Johnston-Peck, M. Cargnello

11:00 CATL 462. Kinetics modeling enabled parameterization and discrimination of nanoparticle surface reactivity evaluated by chemical assays. **X. Bi**, P.K. Westerhoff

11:20 CATL 463. Early-stage catalytic behavior of ethane dehydroaromatization over zinc modified HZSM-5 catalyst via transient kinetic methods. **Y. Xiang**

Section B
Hampton Inn & Suites Convention Center
Riverside I

Unconventional Catalysis Targeting Stable Molecules
Cosponsored by ENFL, ENVR, INOR and PHYS
C. Wang, *Organizer*
C.L. Marshall, *Organizer, Presiding*
C. Wang, *Presiding*

9:00 CATL 464. Biomimetic oxidation catalyst from polymer-nanocrystal composite material. **A. Riscoe**, C. Wrasman, A. Hoffman, A. Menon, A. Boubnov, E. Goodman, S.R. Bare, M. Cargnello

9:20 CATL 465. Conversion of light alkanes to alkyl esters and chlorides using iodine oxides and chlorides: Radical versus non-radical pathways. **T.B. Gunnoe**, J.T. Groves, W.A. Goddard, N. Schwartz, N. Boaz, S.E. Kalman, G. Fortman, R. Fu, R.J. Nielsen, J.M. Goldberg

10:00 CATL 466. Electrochemical carbon dioxide conversion to alcohols. **F. Jiao**

10:40 Intermission.

10:50 CATL 467. Computational searches for energetically efficient CO_2 reduction reaction steps across chemical and materials space. M. Groenenboom, K. Saravanan, Y. Basdogan, **J.A. Keith**

11:30 CATL 468. Highly efficient functionalized porous UiO-66 based metal organic frameworks (UiO66-MOFs) as catalysts for cross coupling reactions. **P. Elumalai**, S.T. Madrahimov

Section C
Hampton Inn & Suites Convention Center
Riverside III

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Cosponsored by ENFL, ENVR and INOR
J. Choi, O. Gazit, M. Kidder, *Organizers*
A. Lepore, *Presiding*

9:00 CATL 469. Catalytic conversion of lignocellulosic feedstock to hydrocarbon fuel intermediates. **A. Padmaperuma**, M. Lilga

9:20 CATL 470. Computational study of aerobic oxidation of 4-(Hydroxymethyl) phenol (4-HMP) by Co(salen). **V. Nziko**, R.C. Johnston, A. Ivanov, T.J. Elder, A. Rudie, D. Turpin, S. Alam, J.J. Bozell, J.M. Parks

9:40 CATL 471. Withdrawn

10:00 CATL 472. Insights into glucosidic bond activation by paired metal chlorides in ionic liquid. **Y. Yang**, Z. Zhang, H. Li, P. Yan

10:20 Intermission.

10:40 CATL 473. Catalytic influence of naturally occurring salts on biomass pyrolysis chemistry: A combined experimental and DFT study. **J.S. Arora**, K. Ansari, P.J. Dauenhauer, S. Mushrif

11:00 CATL 474. Hydrodeoxygenation reaction network of furylmethane oxygenates to jet and diesel range fuels: Probing the role of supported palladium catalyst and hafnium triflet promoter. **S. Dutta**, B. Saha, D.G. Vlachos

11:20 CATL 475. Catalytic conversion of natural cotton fibers to carbon nanotubes and nitrogen functionalization. **G. Zhao**, F. Gao, K. Li, Z. Wang, M. Jahan

Section D
Hampton Inn & Suites Convention Center
Bienville

General Catalysis

A. Savara, *Organizer*
M. Dixit, *Presiding*

8:00 CATL 476. Stereoinversion of *R*-configured secondary alcohols using a single enzymatic approach. **M.M. Musa**, I. Karume, M. Takahashi, S.M. Hamdan

8:20 CATL 477. Extremely fast olefin metathesis in aqueous media with 3rd generation Grubbs-type catalysts. A. Ashcraft, S. Balof, C. Jones, **H.J. Schanz**

8:40 CATL 478. Investigating the oxygen reduction reaction on inorganic/organic interfaces. **M. Anand**, S. Siahrostami, J.K. Norskov

9:00 CATL 479. Novel copper *N*-tosyl nitrenes from bis(pyrazolyl)methane ligands: Investigation of their reactivity towards catalysis. **J. Moegling**, A. Hoffmann, N. Orth, B. Venderbosch, R. Rampmeier, I. Ivanovic-Burmazovic, M. Tromp, S. Herres-Pawlis

9:20 CATL 480. Withdrawn

9:40 Intermission.

10:00 CATL 481. Transition metal nitrides for oxygen electrocatalysis. **H. Abroshan**, P. Bothra, A. Kulkarni, J.K. Norskov, S. Siahrostami

10:20 CATL 482. Calculations on water oxidation catalysis modify the expected mechanism from experiments. **A. Poater**, M. Solà, J. Luque-Urrutia

10:40 CATL 483. Doping carbon catalysis for oxygen reduction reaction. M. Liu, T. Fan, **Y. Liu**, Y. Min

11:00 CATL 484. Unconventional binary ZnO/ZrO_2 heterogeneous catalysts for direct dehydrogenation of isobutane to isobutene. **Y. Liu**, **M. Ke**

11:20 CATL 485. Direct 3D printing of catalytically active structures. **J. Manzano**, Z.B. Weinstein, A.D. Sadow, I.I. Slowing

11:40 CATL 486. Hydrogen-assisted synthesis of CeO_2-Al_2O_3 with enhanced oxygen vacancy density. **B. Chen**

Section E
Hampton Inn & Suites Convention Center
Fulton

Control of Zeolite Structure, Composition & Sites for Catalysis
Cosponsored by INOR
R. Gounder, W.F. Schneider, *Organizers*
S. Goel, *Organizer, Presiding*
D. Hibbitts, *Presiding*

8:00 CATL 487. Materials based on halloysite nanotubes with structured mesoporous silica for sulfur reduction in fluid catalytic cracking. **A.P. Glotov**, N. Levshakov, B. Anikushin, A. Vutolkina, S. Lysenko, E. Ivanov, V. Vinokurov, Y.M. Lvov

8:20 CATL 488. Self-assembly of ZSM-5/SBA-16 with different morphologies and its hydrodesulfurization of dibenzothiophene and 4,6-dimethyldibenzothiophene. X. Wang, Z. Zhao, P. Zheng, J. Fan, **A. Duan**, C. Xu

8:40 CATL 489. Synthesis of mesoporous zeolites using nanocellulose as an inexpensive hard template. **T. Pilyugina**, S.L. Kobaslija, J. Obrien, B.S. Hanna, S.C. Hayden, S. Fernandez

9:00 CATL 490. Control over the mesoporosity of zeolites for the improved accesibility to their acid sites. N. Linares, E. De Oliveira Jardim, E. Serrano, **J. Garcia Martinez**

9:20 Intermission.

9:40 CATL 491. Synthesis protocols for the encapsulation of active and stable Au, AuPt, and AuPd nanoparticles within the protected void environment of zeotypes. **T. Otto**, S.I. Zones, E. Iglesia

10:00 CATL 492. Synthesis and characterization of tin, tin/aluminum, and tin/boron containing MFI zeolites. **M. Shahami**, R. Ransom, D.F. Shantz

10:20 CATL 493. Consequences of zeolitic vs. amorphous supports on the catalytic activity and stability of Ti(IV) and Fe(III) centers. **N. Grosso Giordano**, A.J. Yeh, M. Aigner, C. Shroeder, A. Solovyov, A. Okrut, N. Marinković, H. Koller, S.I. Zones, A.S. Katz

10:40 CATL 494. Synthesis and growth kinetics of zeolite SSZ-39. **R. Ransom**, J. Coote, R. Moulton, F. Gao, D.F. Shantz

Section F
Hampton Inn & Suites Convention Center
Cottonmill

General Catalysis

A. Savara, *Organizer*
S. Kattel, *Presiding*

8:00 CATL 495. CO_2 hydrogenation to CH_3OH on Cu/oxide catalysts. **S. Kattel**, J.G. Chen, P. Liu

8:20 CATL 496. Design of ionic polymer catalysts for the synthesis of cyclic carbonates from CO_2 and epoxides. **F.D. Bobbink**, P. Dyson

8:40 CATL 497. Hierarchically porous monoliths for fixed bed catalysis. **M.G. Bakker**

9:00 CATL 498. Catalytic performance of different zeolite catalysts for oligomerization of 1-butene. **Z. Lei**, M. Ke

9:20 CATL 499. Feasible synthesis of hydroxyapatite-supported palladium nanoparticles with controllable size and distribution and their enhanced catalytic activity. **X. Zhang**

9:40 CATL 500. Deep hydrodesulfurization over nickel phosphide on modified alumina supports. **M.E.**

‡*Cooperative Cosponsorship*

Bussell, C.E. Miles, T. Clinkingbeard, B.J. Morgan, P.J. Topalian

10:00 Intermission.

10:20 CATL 501. Homogenous Pd catalysis for enantioselective intermolecular hydrofunctionalizations of 1,3-dienes. **N.J. Adamson**, S. Malcolmson

10:40 CATL 502. Iridium versus iridium: Nanoparticle and molecular catalysts carrying the same ligand behave differently. **I. Cano**, P.W. van Leeuwen

11:00 CATL 503. Withdrawn

11:20 CATL 504. Leveraging interstitial boron atoms to tailor the acid-base properties of MgO for selective aldol-condensation of acetaldehyde. T. Pham, L. Zhang, D. Shi, M. Komarneni, M. Ruiz-Ramiro, D.E. Resasco, **J. Faria**

THURSDAY AFTERNOON

Section A
Hampton Inn & Suites Convention Center
Antonine

Elucidation of Mechanisms & Kinetics on Surfaces
Cosponsored by COLL, ENVR and PHYS
L. Baker, S. Laursen, *Organizers*
A. Savara, *Organizer, Presiding*

1:00 CATL 505. Acidity as reactivity descriptor for methanol oxidation and dehydration over polyoxometalates. **T. Wilke**, M.A. Barteau

1:20 CATL 506. Withdrawn

1:40 CATL 507. Mechanism of water splitting catalysed by Co-intercalated birnessite studied by SCAN metaGGA. **J. Ning**, R. Remsing, D.R. Strongin, J. Sun

2:00 Intermission.

2:20 CATL 508. Spectroscopic analysis of active sites for electrocatalytic water oxidation in disordered iron-cobalt oxides. **R.D. Smith**, H. Dau

2:40 CATL 509. Predictive catalyst design on alloy nanoparticle supported graphene for ORR. **T. Lozano**, R. Rankin

3:00 CATL 510. Ligand-regulated ORR activity of Au nanoparticles in alkaline medium: The importance of surface coverage of ligands. **L. Lu**, S. Zou, J. Fan

3:20 CATL 511. Vibrationally excitated CO_2 desorbed from decomposition of formate on Cu(111). F. Muttaqien, H. Oshima, Y. Hamamoto, K. Inagaki, I. Hamada, **Y. Morikawa**

3:40 CATL 512. Phosphorus-doped and lattice-defective carbon as metal-like catalyst for selective hydrogenation of nitroarenes. **G. Ruijie**, J. Zou, L. Pan

Section B
Hampton Inn & Suites Convention Center
Riverside I

New Techniques & Applications of Magnetic Resonance Methods in Heterogeneous Catalysis

F.A. Perras, S.L. Scott, *Organizers*
N. Washton, *Organizer, Presiding*

1:00 CATL 513. Solid-state NMR of metals and halogens in catalysts their precursors. **R.W. Schurko**, C. O'Keefe, M. Hildebrand, K. Johnston, L. O'Dell, A.J. Rossini

1:40 CATL 514. *In-situ* NMR of the catalytic depolymerization of lignin model polymers. **M.B. Foston**, S.L. Scott, D.W. Hoyt, N. Washton

2:00 CATL 515. *Operando* solid-state NMR spectroscopy for biomass conversion with solid catalysts. **L. Qi**, A. Chamas, D.W. Hoyt, E.D. Walter, N. Washton, S.L. Scott

2:20 CATL 516. Real-time monitoring of catalysis to extremophiles: High pressure – high temperature MAS-NMR of mixed phase samples. **D.W. Hoyt**

2:40 Intermission.

3:00 CATL 517. Solid-state NMR spectroscopy for the comprehensive structural and dynamic characterization of covalently bound and surface-adsorbed catalysts. **J. Bluemel**

3:40 CATL 518. Magic angle spinning solid-state NMR spectroscopy of impregnated heterogeneous catalysts. R.L. Johnson, T. Pfennig, M.P. Hanrahan, M.J. Ryan, B.H. Shanks, **A.J. Rossini**

4:00 CATL 519. Parahydrogen spin labelling studies of hydrogenation catalysis over silica-encapsulated Pt-Sn intermetallic nanoparticles. E.W. Zhao, R. Maligal Ganesh, W. Huang, **C.R. Bowers**

4:20 CATL 520. Capturing CO_2 with metal organic frameworks. **J.A. Reimer**

Section C
Hampton Inn & Suites Convention Center
Riverside III

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Cosponsored by ENFL, ENVR and INOR
J. Choi, O. Gazit, M. Kidder, *Organizers*
A. Lepore, *Presiding*

1:00 CATL 521. Hydrothermally stable Ru-TiO_2 catalyst for the decarboxylative coupling of acetic acid in aqueous environments. N. Aranda-Pérez, M. Ruiz-Ramiro, J. Echave, **J. Faria**

1:20 CATL 522. Carbonyl hydrogenation over atomically dissperesd precious metals on alumina. **A. Lepore**, Z. Li

1:40 CATL 523. Kinetics of lignin monomer production from poplar wood by reductive catalytic fractionation. **E. Anderson**, M. Stone, M. Huelsey, G. Beckham, Y. Roman-Leshkov

2:00 CATL 524. Lignin depolymerization over supported mono-(Ni, Ru) and bimetallic (Ni-Ru) nanoparticles. **M. Zaheer**

2:20 Intermission.

2:40 CATL 525. Group IB metal activated anatase TiO_2 for selective catalytic deoxygenation. **Z. Zhang**, J. Mao, K. Liu, X. Zhang, Q. Fang, P. Yan, G. Hou, S. Bai, X. Guo

3:00 CATL 526. Effect of space velocity and long residence time on Fischer Tropsch products and catalyst reduced with different gases. **J. Gorimbo**, A. Muleja

Section D
Hampton Inn & Suites Convention Center
Bienville

General Catalysis

A. Savara, *Organizer*
M. Dixit, *Presiding*

1:00 CATL 527. Understanding single molecule pro-catalyst "activation" for growth of carbon nanotubes. **G. Esquenazi**, A.R. Barron

1:20 CATL 528. Palladium dendron encapsulated nanoparticles supported on MCM-41 and SBA-15. **Y. Lou**, D.F. Shantz

1:40 CATL 529. Catalytic vinylidene C(sp^2)–H insertion using a dinuclear catalyst. **T. Steiman**, C. Uyeda

2:00 CATL 530. Synthesis of glycerol oligomers from etherification of glycerol in presence of zeolite-supported calcium catalysts. C. Chen, **B. Chen**

2:20 CATL 531. Knowledge driven catalyst screening using *In-situ* far infrared spectroscopy. **H. Li**, P. Yan, Z. Zhang

2:40 CATL 532. Withdrawn

3:00 Intermission.

3:20 CATL 533. Designing carbon-based materials for effective electrochemical reduction of CO_2. **S. Siahrostami**, K. Jiang, C. Kirk, M. Karamad, K. Chan, H. Wang, J.K. Norskov

3:40 CATL 534. Pt clusters supported single Fe atoms for preferential oxidation of CO in the excess of H_2 with wide operation temperature window. **Y. Lou**, J. Liu

4:00 CATL 535. Withdrawn

Section E
Hampton Inn & Suites Convention Center
Fulton

Control of Zeolite Structure, Composition & Sites for Catalysis
Cosponsored by INOR
R. Gounder, W.F. Schneider, *Organizers*
S. Goel, *Organizer, Presiding*
D. Hibbitts, *Presiding*

1:00 CATL 536. Hydride transfer versus deprotonation kinetics in the isobutane-propene alkylation reaction: A computational study. **C. Liu**, R.A. Van Santen, E. Hensen, E. Pidko

1:20 CATL 537. Conversion of methanol to hydrocarbons over H-ZSM-5 zeolite-reaction pathway is related to the framework aluminum siting. **T. Liang**, J. Wang, Y. Xiang

1:40 CATL 538. Direct detection of multiple acidic proton sites in zeolite HZSM-5. **K. Chen**, M. Abdolrahmani, J.L. White

2:00 CATL 539. Oligomerization of ethylene to select oligomers on Ni^{2+}-containing ETS-10. J. Thakkar, X. Yin, **X. Zhang**

2:20 Intermission.

2:40 CATL 540. Mechanistic investigation of dissociation of β-O-4 linkage in the presence of solvent on MWW-2D zeolite framework. **V. Jain**, N. Rai

3:00 CATL 541. The role of anharmonicity in the confinement effect in zeolites: Structure, spectroscopy and adsorption free energy of ethanol on H-ZSM-5 in aqueous phase. **M. Lee**, Y. Wang, V. Glezakou, R. Rousseau

3:20 CATL 542. Cis-trans isomerism and the role of dilution in organic structure direction to relevant zeolite catalysts AEI (SSZ-39) and GME (CIT-9). **M. Dusselier**, J. Kang, D. Xie, M.E. Davis

3:40 CATL 543. Reveal and tailor mesoporous ZSM-5 synthesis in a new solid crystallization route. Y. Wang, N. Baxter, **S. Wang**

Section F
Hampton Inn & Suites Convention Center
Cottonmill

General Catalysis

A. Savara, *Organizer*
S. Kattel, *Presiding*

1:00 CATL 544. Ionic liquid-assisted synthesis of nanoscale (MoS2) x(SnO2)1−x on reduced graphene oxide for the electrocatalytic hydrogen evolution reaction. **S. Ravula**, C. Zhang, J.B. Essner, J.D. Robertson, J. Lin, G.A. Baker

1:20 CATL 545. Role of oxygen vacancies in hydrogenation reaction on non-precious metal oxides: experiment and DFT studies. **Y. Zhang**, X. Zhang, J. Zou

1:40 CATL 546. Withdrawn

2:00 CATL 547. Sodium tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (NaBArF) catalyzed Friedel-Crafts addition reactions and mechanistic studies. **K. Mesa**, H. Hibbard, A.K. Franz

2:20 CATL 548. On the structural reconstruction and catalytic origins of electrocatalytic single atom catalysts. **G. Wan**, H. Chen, T. Li, J. Shi

2:40 CATL 549. Hydrodenitrogenation of quinoline over β- Al_2O_3 supported Pt catalysts. **J. Liu**, **W. Li**, X. Gao, Z. Luo

3:00 Intermission.

3:20 CATL 550. Withdrawn

3:40 CATL 551. On the mechanism of the titanium catalyzed redox formal [2+2+1] catalytic formation of pyrroles. **Z.W. Gilbert**, I. Tonks

4:00 CATL 552. Carbon dioxide reduction by methane through dry reforming reaction. **C. Zhang**

4:20 CATL 553. Effect of molecular size on the HDS mechanism over different MoS_2 active sites: A DFT study. **P. Zheng**, Y. Li, C. Xiao, D. Hu, A. Duan, L. Zhao

‡*Cooperative Cosponsorship*

CELL

Division of Cellulose & Renewable Materials

M. Roman, *Program Chair*

SUNDAY MORNING

Section A
Loews New Orleans Hotel
LaFourche/Pointe Coupee

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Cosponsored by BIOL, BIOT and POLY
U.P. Agarwal, R.H. Atalla, H. Chanzy, A. Isogai, *Organizers*
A.D. French, S. Renneckar, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 1. Structural heterogeneity and matrix polysaccharide interactions of cellulose in plant cell walls from multidimensional solid-state NMR. P. Phyo, T. Wang, **M. Hong**

8:30 CELL 2. Withdrawn

8:55 CELL 3. Revisit of microfibril structure diversity in higher plants. **Y. Nishiyama**, T. Kuribayashi, Y. Ogawa

9:20 CELL 4. Nematic structuring of transparent and multifunctional nanocellulose papers. M. Zhao, F. Ansari, M. Takeuchi, M. Shimizu, **T. Saito**, L. Berglund, A. Isogai

9:45 Intermission.

10:00 CELL 5. Accessibility of hydroxyl groups related to cellulose aggregation. **L. Salmén**

10:25 CELL 6. Manufacturing high performance cellulose fibres from solution. **S.J. Eichhorn**, C. Zhu, A. Koutsomitopoulou, K.D. Potter

10:50 CELL 7. Morphological and structural analysis of cellulose microfibrils using enzymatic treatment. **N. Hayashi**

11:15 CELL 8. Real-time visualization of lignin structure during dilute acid pretreatment of native and lignin mutants of switchgrass and poplar. **S. Pingali**, H.M. O'Neill, L. Petridis, M.B. Foston, B. Evans, A. Ragauskas, J. Smith, B.H. Davison, V. Urban

Section B
Loews New Orleans Hotel
St. Landry

New Horizons in Sustainable Materials

Financially supported by Elsevier–Carbohydrate Polymers; The Center for Renewable Carbon–University of Tennessee; Department of Sustainable Biomaterials–Virginia Tech; School of Forest Resources, University of Maine
S.M. Murphy, M. Roman, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 9. Renewable fuels and materials from plant biomass: Are we there yet?. **N. Sathitsuksanoh**

8:30 CELL 10. Integrated biorefinery approach to produce biosugar from lignocellulosic biomass. **S. Park**

8:55 CELL 11. Sustainable catalytic transformations to produce renewable soft materials. **S.C. Chmely**

9:20 CELL 12. The hybrid conversion of lignin into biodiesel. **M.B. Foston**

9:45 Intermission.

10:00 CELL 13. Anisotropic composite foams from lignocellulosic biomass: Mechanical and thermal properties. **N. Lavoine**, V. Apostolopoulou Kalkavoura, L. Bergstrom

10:25 CELL 14. Nanocellulose/polymer composite microparticles prepared by emulsion-templated synthesis. **S. Fujisawa**, E. Togawa, K. Kuroda

10:50 CELL 15. Detection of human neutrophil elastase with fluorescent peptide sensors conjugated to TEMPO oxidized nanocellulosic foams. **K.R. Fontenot**, V. Edwards

11:15 CELL 16. Bio-based intumescent flame retardant coating for nylon-cotton fabric based on synergistic combination of tannic acid and phytic acid. **Z. Xia**, S. Yu, W. Kiratitanavit, J. Kumar, R. Mosurkal, R. Nagarajan

Section C
Loews New Orleans Hotel
St. Tammany

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Cosponsored by AGFD, ANYL and CARB
H. Kamitakahara, C. Wong, *Organizers*
G. Boons, A. Dell, L.C. Hsieh-Wilson, J.C. Paulson, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 17.
Recent advance in chemoenzymatic glycoprotein synthesis. **L. Wang**

8:30 CELL 18. Sugars & proteins: Exploring and exploiting sugar chemical biology. **B.G. Davis**

8:55 CELL 19. Analysis of glucose mediated glycoprotein folding events in the endoplasmic reticulum. **Y. Ito**

9:20 CELL 20. O-GlcNAc glycosylation: From reductionism to systems biology. **L.C. Hsieh-Wilson**

9:45 Intermission.

10:00 CELL 21. Hyphenated IM-MS methods as high-resolution sequencing tools for carbohydrates. **S. Flitsch**

10:25 CELL 22. Hybridation of mass spectrometry and laser spectroscopy: A new technology for glycoanalytics. **I. Compagnon**

10:50 CELL 23. Withdrawn

11:15 CELL 24. Glycan spatial sequencing with regio-specific spectral documentation. **V.N. Reinhold**

Section D
Loews New Orleans Hotel
Beauregard

Failed Brilliance in Nanocellulose Science & Technology
Cosponsored by ANYL
E. Kontturi, *Organizer*
A. Bismarck, K. Lee, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 25. Withdrawn

8:30 CELL 26. Grafting density design of surface-modified nanocellulose for polymer composites. **H. Soeta**, T. Saito, L. Berglund, A. Isogai

8:55 CELL 27. Emulsibility and stability mechanism of oil in water emulsion with TEMPO-oxidized cellulose nanofibers. **Y. Goi**, T. Saito, A. Isogai

9:20 CELL 28. From polymer to surface stabilisation of cellulose in ionic liquids. G.J. Partl, J.K. Helminen, D. Rico del Cerro, V. Mäkelä, E. Kontturi, I.A. Kilpeläinen, **A. King**

9:45 Intermission.

10:00 CELL 29. Withdrawn

10:25 CELL 30. Iridescent security planchettes, silicone rubber molds and *pseudopapilionoides cellulosae*. T. Abitbol, A. Blonder, J. Budman, **D.G. Gray**, O. Shoseyov, S. Shoval

10:50 CELL 31. Included? Not included! (Nano)Cellulose inclusion compounds. A. Mautner, K. Lee, E. Kontturi, **A. Bismarck**

11:15 CELL 32. Turning "nano"dreams into "mega"nightmares: How the expectations of academic and industrial R&D players on nanocellulose could be frustrated by polices and regulations on nanotechnologies in Europe. **D. Da Silva Perez**

Section E
Loews New Orleans Hotel
Terrebonne

Wood-Based Materials for Energy & Water

Nanocellulose-Based Technologies

Cosponsored by ENFL, ENVR and MPPG
L. Hu, L. Nyholm, L. Wagberg, J. Zhu, *Organizers*
S. Lee, Z. Ren, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 33. Fluorogenic sensing of water diffusion and its effects in CNC based composites. **S. Seethamraju**, J.W. Woodcock, R. Beams, S. Stranick, J.W. Gilman

8:30 CELL 34. Strategies towards tough, stiff and strong poly(lactic acid) composites. **X. Meng**, H.L. Tekinalp, S. Ozcan

8:55 CELL 35. Cellulose nanocrystals grafted with Poly(glycidyl methacrylate) for their compatibilization in nanocomposites. **M. Le Gars**, M. Ji, H. Salmi, N. Belgacem, P. Roger, J. Bras

9:20 CELL 36. Modification of cellulose nanocrystals with semiconducting polymers. A. Chang, S. Chen, **K.R. Carter**

9:45 Intermission.

10:00 CELL 37. Intelligent paper: Printed electronics on advanced cellulosic nanomaterials. **B. Kippelen**

10:25 CELL 38. Nanocellulose based energy storage devices. Z. Wang, P. Tammela, M. Strömme, **L. Nyholm**

10:50 CELL 39.
Exploring the potential of cellulose nanofibrils in energy and environmental applications. **F. Jiang**, L. Hu

11:15 CELL 40. Wood-derived cellulose nanopaper simultaneously with enhanced transparency and a self-cleaning superhydrophobic surface. **S. Chen**, Y. Song, F. Xu

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Energy, Water & Food Production
Sponsored by AGFD, Cosponsored by CELL, GEOC and MPPG

Bioenergy & Bio-Based Chemicals
Sponsored by ENFL, Cosponsored by CELL

SUNDAY AFTERNOON

Section A
Loews New Orleans Hotel
LaFourche/Pointe Coupee

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Cosponsored by BIOL, BIOT and POLY
U.P. Agarwal, R.H. Atalla, H. Chanzy, A. Isogai, *Organizers*
T. Saito, L. Salmén, *Presiding*

1:05 CELL 41. Small-angle scattering methods for efficient characterization of wood nanostructure and moisture behavior. **P.A. Penttilä**, L. Rautkari, M.K. Osterberg, R. Schweins

1:30 CELL 42. In situ measurement of cellulose biosynthesis using small angle X-ray scattering. H. Tajima, P.A. Penttilä, K. Yamamoto, Y. Yuguchi, J. Sugiyama, **T. Imai**

1:55 CELL 43.
Characterization of electrospun nanofibers composed of water soluble xylans. J. Duan, M. Karaaslan, M. Cho, L. Liu, A.M. Johnson, **S. Renneckar**

2:20 CELL 44. Frequency filtered molecular dynamics trajectory compared with crystallographic temperature factor in highly crystalline chitin. **Y. Ogawa**, Y. Nishiyama, K. Mazeau

2:45 Intermission.

3:00 CELL 45. Visualization of freeze-fixed distribution of monolignol glucosides in plants. D. Aoki, Y. Matsushita, **K. Fukushima**

3:25 CELL 46. Chomophores from hexeneuronic acids (HexA) – identification of structures, formation mechanisms, and destruction by peroxide bleaching. **T. Rosenau**, A. Potthast, T. Hosoya, N. Zwirchmayr, T. Dietz

3:50 CELL 47. Desorption behavior of guest molecule from cellulose I-EDA complex crystals: Molecular dynamics study. **T. Yui**, T. Uto

4:15 CELL 48. Atomic level structure characterization of carbohydrate pre and post lignin treatment by dynamic nuclear polarization: Enhanced solid state NMR. **H. Luo**

‡*Cooperative Cosponsorship*

Section B
Loews New Orleans Hotel
St. Landry

New Horizons in Sustainable Materials

Financially supported by Elsevier–Carbohydrate Polymers; The Center for Renewable Carbon–University of Tennessee; Department of Sustainable Biomaterials–Virginia Tech; School of Forest Resources, University of Maine
S.M. Murphy, M. Roman, *Organizers, Presiding*

1:05 CELL 49. Toward carbon fibers from single component Kraft lignin systems: An application of green chemistry with forest biomaterials. **S.V. Patil**, H. Sadeghifar, S. Sen, J. Zhu, D. Argyropoulos

1:30 CELL 50. Clicking lignin towards functional renewable materials. **Y. Habibi**

1:55 CELL 51. Gelatin hydrogel actuators. **L. Hanzly**, J.R. Barone

2:20 CELL 52. Interactions at biopolymer blend thin films. **K. Niegelhell**, M. Süssenbacher, J. Sattelkow, K. Zhang, H. Plank, T. Mohan, **S. Spirk**

2:45 Intermission.

3:00 CELL 53. Bacterial NanoCellulose: closer to the market. **M. Gama**, F. Dourado

3:25 CELL 54. Highly porous and highly permeable bacterial cellulose nanopaper as reinforcement for polymers. A. Santmarti, M. Hervy, A. Mautner, A. Kondor, A. Bismarck, **K. Lee**

3:50 CELL 55. Length distributions of nanocelluloses can be evaluated by rheological measurements of their dispersions. **R. Tanaka**, Y. Kashiwagi, T. Inoue

4:15 CELL 56. Nanocellulose for nanotechnologies. **L. Hu**

4:55 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Cosponsored by AGFD, ANYL and CARB
H. Kamitakahara, C. Wong, *Organizers*
M. Aebi, B.G. Davis, Y. Ito, A. Planas, *Presiding*

1:05 CELL 57. Concepts of N-linked protein glycosylation. **M. Aebi**

1:30 CELL 58. Homogeneous N-glycoprotein containing a common glycan structure for the improvement of antibody-based therapeutics. **N. Lin**

1:55 CELL 59. Systematic synthesis of glycosaminoglycan oligosaccharides. **J. Tamura**

2:20 CELL 60. Regioselective derivatizations of *E. coli* chondroitin polysaccharide through tailored multi-step procedures. **E. Bedini**

2:45 Intermission.

3:00 CELL 61. Propelling chemically modified glycosaminoglycans into the clinic. **G.D. Prestwich**

3:25 CELL 62. Protection-free direct anomeric activation for key glycosyl intermediates. **S. Shoda**, M. Noguchi, G. Li

3:50 CELL 63. Understanding and engineering the deacetylation pattern of chitin deacetylases. **A. Planas**

4:15 CELL 64. Pectins–are they polysaccharides, proteoglycans, glycan domains of multi-glycan polymers, or all three? Evidence from studies of pectic homogalacturonan biosynthetic galacturonosyltransferases and mutants/transgenics thereof. **D. Mohnen**, M.A. Atmodjo, A.K. Biswal, L. Tan, K. Engle, R.A. Amos

Section D
Loews New Orleans Hotel
Beauregard

Assembly & Colloidal Interactions of Cellulose Nanocrystals
Cosponsored by COLL
Financially supported by EPNOE
C. Schütz, *Organizer*
W. Thielemans, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL 65. Probing assembling and aggregation of cellulose nanocrystals at the nanoscale using small angle scattering. Y. Liu, D. Stoeckel, K. Gordeyeva, C. Schütz, **A.B. Fall**, L. Bergstrom

1:30 CELL 66. Cellulose-based multifunctional photonic structures. **G. Guidetti**, A. Espinha, B. Frka-Petesic, S. Atifi, M.C. Serrano, A.G. Dumanli, A. Blanco, W.Y. Hamad, C. Lopez, S. Vignolini

1:55 CELL 67. Bimodal cellulose nanocrystal blends for bioinspired damage tolerant photonic films. **B. Natarajan**, A. Krishnamurthy, C.D. Emiroglu, X. Qin, A. Forster, D. Fox, J. Foster, C. Weder, J. Obrzut, S. Keten, J.W. Gilman

2:20 CELL 68. Controlling the diffraction of light by cellulose nanocrystal assemblies using electric or magnetic fields. **B. Frka-Petesic**, G. Guidetti, G. Kamita, H. Radavidson, B.R. Jean, L. Heux, S. Vignolini

2:45 Intermission.

3:00 CELL 69. Controlling the deposition pattern of cellulose nanocrystals in drying droplets using internal flow fields. A. Gencer, C. Schütz, **W. Thielemans**

3:25 CELL 70. Development of nanoparticle alignment regimes in drying cellulose nanocrystal droplet suspensions for additive manufacturing. **C. Pritchard**, F. Navarro-Arzate, M. Roman, M. Bortner

3:50 CELL 71. Hierarchical self-assembly of cellulose in a confined geometry. **R. Parker**, B. Frka-Petesic, G. Guidetti, G. Kamita, T. Zhao, S. Vignolini

4:15 CELL 72. Rheology and application of cellulose nanocrystal inks for direct ink writing. **M. Hausmann**, G. de Freitas Siqueira, R. Libanori, D. Kokkinis, P. Rühs, T. Zimmermann, A. Studart

Section E
Loews New Orleans Hotel
Terrebonne

Wood-Based Materials for Energy & Water

Wood-Fiber & Wood-Scaffold Based Technologies

Cosponsored by ENFL, ENVR and MPPG
L. Hu, S. Lee, L. Nyholm, Z. Ren, J. Zhu, *Organizers*
L. Wagberg, *Organizer, Presiding*
F. Jiang, *Presiding*

1:05 CELL 73.
Polydopamine assisted Cu NPs deposition on biomass substrates for flexible, wearable and self-cleaning electronics. **X. Wang**, Y. Yang, Q. Huang

1:30 CELL 74. Environmentally sound textile dyeing technology with nanofibrillated cellulose. **Y. Kim**, L. McCoy, E. Lee, H. Lee, R. Saremi, C. Feit, I. Hardin, S. Sharma, S. Mani, S. Minko

1:55 CELL 75. Paper fines as renewable source for supercapacitor electrode materials. **M.A. Hobisch**, E. Mourad, W. Fischer, A. Zankel, A. Mautner, S. Freunberger, R. Eckhart, W. Bauer, S. Spirk

2:20 CELL 76. Structural design of cellulose paper composites for green chemistry and electronics. **H. Koga**

2:45 Intermission.

3:00 CELL 77. Conductive wood membrane electrode for energy recovery from wastewater treatment. **Z. Ren**, Z. Huang, A. Gong, L. Hu

3:25 CELL 78. Functional lignocellulosic materials for water purification applications. **E. Cabane**, M. Vidiella del Blanco, S. Vitas

3:50 CELL 79. Modification of transparent wood for photonics functions. **L. Berglund**, Y. Li, Q. Fu, S. Popov, I. Sychugov, M. Yan

4:15 CELL 80. Energy storage and energy generation based on the materials and structures derived from wood. **H. Zhu**, A. Mukhopadhyay, L. Yang

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

Bioenergy & Bio-Based Chemicals
Sponsored by ENFL, Cosponsored by CELL

Energy, Water & Food Production
Sponsored by AGFD, Cosponsored by CELL, GEOC and MPPG

Plant Omics
Sponsored by ANYL, Cosponsored by CELL and MPPG‡

SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

General Posters

M. Roman, *Organizer*

7:00–9:00

CELL 81. Modification of cellulose with methyl ester through transesterification reaction in imidazolium carboxylates. **S.B. Kusuma**, S. Nomura, M. Yamaguchi, D. Hirose, Y. Yasaka, K. Ninomiya, K. Takahashi

CELL 82. CO_2 adsorbent material based on cellulose nanofibrils derived from agricultural wastes. F. Valdebenito, G. Ciudad, G. Chinga-Carrasco, **Y. Habibi**

CELL 83. Cellulose-cyclodextrin co-polymer for removal of microcystin on water remediation. **D. Gómez Maldonado**, M.N. Hornus, B. Vega, I. Filpponen, A. Wilson, M. Waters, M. Peresin

CELL 84. Withdrawn

CELL 85. Enhancing in situ hydrogen peroxide generation of greige cotton nonwoven wound dressings via ascorbate stabilized copper micro- and nano-particles. **N.T. Prevost**, V. Edwards, B.D. Condon, D. Yager

CELL 86. Design, preparation and activity of intelligent cellulose-based protease sensor & modulating/fibroblast promoting (PROTOS-FIBRO) dressings. **V. Edwards**, K.R. Fontenot, N.T. Prevost, D. Yager, F. Liebner, B.D. Condon

CELL 87. Withdrawn

CELL 88. Nano-emulsions and nano-latexes stabilized by hydrophobically functionalized cellulose nanocrystals. **Y. Zhang**, V. Karimkhani, B.T. Makowski, G. Samaranayake, S.J. Rowan

CELL 89. Tannin micro- and nanocapsules for storage and controlled delivery of hydrophobic molecules. E.D. Bartzoka, **H. Lange**, L. Zongo, P. Mosesso, C. Crestini

CELL 90. Fluid flow in paper-derived silica-polymer hybrids. **N. Herzog**, M. Gallei, T. Meckel, M.A. Biesalski, A. Andrieu-Brunsen

CELL 91. Cationic starch as strengthening agent in nanofibrillated and bacterial cellulose nanopapers. **M. Hervy**, P. Lahtinen, T. Tammelin, K. Lee

CELL 92. Cellulose nanofibrils production using deep eutectic solvents and twin screw extrusion. H. Spieser, F. Rol, F. Bardot, V. Meyer, **J. Bras**

CELL 93. The role of residual lignin in lignin containing cellulose nanofibrils (L-CNF). **M.C. Iglesias**, R. Gleisner, J. Zhu, L. Tetard, K. Stana-Kleinschek, C.E. Frazier, M. Peresin

CELL 94. Morphological, chemical, thermal and mechanical effects of cellulose nanocrystals ratios on silk fibroin/cellulose nanocrystals electrospun mats. **S. Sanchez Diaz**, T.J. Elder, A. Restrepo Osorio, O. Fasina, M. Peresin

CELL 95. Synthesis and characterization of nanocrystalline hydroxyapatite derived from eggshell for biomedical applications. **E. Moura**, A. Lodis, P. Reis, R. Wellen

CELL 96. Synthesis and characterization of nanocellulose obtained from pineapple peel wastes. **J. Vega-Baudrit**, M. Camacho, Y. Corrales Ureña, M. Lopretti, G. Moreno

CELL 97. Evaluating the biological response and biodistribution of cellulose nanocrystal nanocomposite hydrogels. **K.J. De France**, M. Badv, J. Dorogin, E.D. Cranston, T. Hoare

‡*Cooperative Cosponsorship*

CELL 98. Continuous composite fiber based on TEMPO-oxidized cellulose nanofibril/chitosan obtained by interfacial polyelectrolyte complexation. **R. Grande**, E. Trovatti, A.J. Carvalho

CELL 99. Tunable surface energy wood-biopolymer macrofibers. **T. Nypelo**, S. Asaadi, G. Kneidinger, H. Sixta, J. Konnerth

CELL 100. Residual wood polymers facilitate compounding of microfibrillated cellulose with poly(lactic-acid) for 3D printer filaments. **A. Winter**

CELL 101. Protein/polysaccharides biocomposite characterization via confocal microscopy. **D.E. Verrill**, A. Morales, S. Brown, S.M. O'Malley, D. Salas-de la Cruz

CELL 102. Different strategies for the preparation of nanocellulose composites with three-dimensional structure. A. Santamaria-Echart, L. Urbina, A. Arbelaiz, A. Retegi, M. Corcuera, **A. Eceiza**

CELL 103. Valorization of hemicellulose hydrolyzates into eco-friendly surfactants. **W. Liu**, M. Roman

CELL 104. New foamed materials from hemicelluloses. **L. Hardelin**, A. Ström, A. Larsson

CELL 105. Food packaging made from chitosan and hemicellulose. **A.M. Johnson**, D. Camacho, H. Jeon, S. Renneckar

CELL 106. Clicking hemicelluloses and nanocellulose toward functional fully biobased materials. L. Puchot, J. Communal, D. Da Silva Perez, **Y. Habibi**

CELL 107. From low-molecular weight hemicelluloses to new biopolymers. **L. Puchot**, D. Da Silva Perez, Y. Habibi

CELL 108. Microwave-assisted extraction of lignin from coconut shell: Insights on the effects of Brønsted and Lewis acids catalysts in the lignin structure. **F. Figueredo-Sobrinho**, M.M. Souza Filho, S.E. Mazzetto, D. Lomonaco

CELL 109. Synthesis and mechanical characterization of high pressure laminates modified with Kraft lignin. M. Taverna, V.V. Nicolau, **D. Estenoz**

CELL 110. Search for production of high quality lignin from technical lignins by enzymatic catalysis. **J. Mikkilä**, J. Kuuskeri, M.R. Mäkelä, J. Kontro, P. Nousiainen, J. Sipila, K. Hildén

CELL 111. Design of a new, accurate laccase activity assay method based on "lignin-like" compounds. **V. Perna**, J. Agger, J. Holck, A.S. Meyer

CELL 112. Ceramic membranes for lignin valorization. S. Schoenherr, D. Humpert, M. Ebrahimi, P. Geigle, S. Demharter, S. Schuetz, F. Ehlen, **P.M. Czermak**

CELL 113. Multiphase materials of lignin and cellulosic mesophases. **M.G. Laborie**, R. Gleuwitz, J. Mao, C. Friedrich

CELL 114. Functionalized lignin as building block for biobased polyurethane foams. **M. Zieglowski**, S. Trosien, M.A. Biesalski

CELL 115. Fractionation of lignin derived compounds from thermochemical processed lignin towards antimicrobial properties. **L. Dodge**, J. Shi, S. Nokes

CELL 116. Microwave-assisted extraction of lignin from water hyacinth (*Eichhornia crassipes*). **P. Sing-udom**, T. Chaisuwan, A. Luengnaruemitchai, S. Wongkasemjit

CELL 117. Real-time measurement of laccase catalyzed formation of radicals in lignin by electron paramagnetic resonance spectroscopy. **L. Munk**, M. Andersen, A.S. Meyer

CELL 118. Lignin based polyurethane foam: Relationship between chemical structure, molecular weight, and foam properties. **L. Liu**, L. Ji, S.C. Patankar, M. Cho, S. Renneckar

CELL 119. Applicability of laccase mediator systems of recombinant laccase catalyzed oxidation of lignin at low pH. **J. Kontro**, P. Nousiainen, M. Kähkönen, U. Hyväkkö, J. Mikkilä, M.R. Mäkelä, K. Hildén, J. Sipila

CELL 120. Mediator supported lignin enzymatic degradation for aromatic production. **L. Longe**, G. Garnier, K. Saito

CELL 121. Application of lignins in phenol formaldehyde adhesive. H. Jameel, **X. Jiang**, F. Zhang, J. Du, H. Chang

CELL 122. Carbonization of electrospun and wetspun lignin based fibers. **T. Hinkel**, **C. Upp**, **A. Bansode**, H. Nam, I. Filpponen, S. Adhikari, M. Auad

CELL 123. Polymer morphology of lignin in carbon fiber precursors from hardwood and herbaceous feedstocks. **V. Garcia-Negron**, O. Hosseinaei, S. Pingali, S.C. Chmely, D.P. Harper

CELL 124. Cellulose-based carbon fiber reinforced polymers: Intensifying interfacial adhesion. **L. Szabo**, S. Imanishi, R. Hoshino, N. Kawashima, D. Hirose, T. Tsukegi, K. Takahashi

CELL 125. Production of functional lignin units as building units with germicidal activity from cereal residues. **M. Lopretti**, G. Lluberas, A. Rodriguez, H. Cerecetto, N. Lecot, J. Vega-Baudrit

CELL 126. Microcapsules and membranes from biorefinery of products of soya industrialization. G. Lluberas, J. Herrera, J. Zygadlo, P. Raimonda, J. Vega-Baudrit, **M. Lopretti**

CELL 127. Thermogravimetric screening of blowing agents for application as an additive in experimental fast pyrolysis of cellulose. **E. Terrell**, M. Garcia Perez

CELL 128. High performance cyanate esters and poly(benzoxazine) from fast pyrolysis of lignocellulosic biomass. **M. Barde**, C.W. Edmunds, N. Labbé, **M.L. Auad**

CELL 129. Synthesis of unsaturated monomers from carbonyl compounds in pyrolytic bio-oil. **M. Barde**, **K. Avery**, C.W. Edmunds, N. Labbé, M. Auad

CELL 130. Effective adsorption and recovery of furfural and 5-hydroxymethylfurfural by cross-linked polyethylenimines. **Q. Yang**

CELL 131. Analysis of the influence of lignocellulose characteristics on thermal behavior using pyrolysis gas-chromatography/mass spectrometry. **S. Hodges**, G. Mortha, C. Dupont, E. Santillan-Jimenez

CELL 132. High value carotenoids from biorefinery waste streams. **M. Vin-Nnajiofor**, J. Shi, L. Das

CELL 133. Oxypropylation of lignocellulosic agro-industrial residues: New approaches and tools towards process optimization. J.A. Pinto, M.A. Prieto, I.C. Ferriera, N. Belgacem, A.E. Rodrigues, **F. Barreiro**

CELL 134. Single crystals of biosynthesized and biodegradable Poly[(R)-3-hydroxybutyrate-*co*-(R)-3-hydroxyhexanoate] (PHBHx). **C. Liu**, I. Noda, D.C. Martin, B. Chase, J.F. Rabolt

CELL 135. Effect of hot water pretreatment in simple pulping utilizing a laboratory scale microwave reactor. **U.T. Hyvakko**, **P. Nousiainen**, P. Kilpeläinen, J. Sipila

MONDAY MORNING

Section A
Loews New Orleans Hotel
LaFourche/Pointe Coupee

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Cosponsored by BIOL, BIOT and POLY
U.P. Agarwal, R.H. Atalla, H. Chanzy, *Organizers*
A. Isogai, *Organizer, Presiding*
K.J. Edgar, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 136. Phase separation and rheological properties of cellulose nanocrystals with different surface charge densities. T. Abitbol, D. Kam, Y. Kalisman, **D.G. Gray**, O. Shoseyov

8:30 CELL 137. Function of the Golgi apparatus in differentiating xylem in *Chamaecyparis obtusa*. **K. Takabe**

8:55 CELL 138. Laccase/TEMPO oxidation in the production of hemicellulose hydro- and aerogels. K. Parikka, I. Nikkilä, **M. Tenkanen**

9:20 CELL 139. Electric and magnetic properties of cellulose nanocrystals in suspension revealed by field-induced birefringence. **B. Frka-Petesic**, J. Sugiyama, B.R. Jean, S. Kimura, H.D. Chanzy, G. Maret, L. Heux

9:45 Intermission.

10:00 CELL 140. Putting a charge into polysaccharides. B.L. Nichols, Y. Dong, **K.J. Edgar**

10:25 CELL 141. Magnetic field induced alignment of cellulose nanocrystals in polyvinyl alcohol suspensions. **M. Wada**, H. Morii, R. Kusumi, F. Kimura, T. Kimura

10:50 CELL 142. Tissue-specific cellulose microfibril assembly patterns in plant cell walls: A study with sum frequency generation microscopy. **S.H. Kim**

11:15 CELL 143. Outstanding toughness of cherry bark achieved by a unique cell wall structure. **K. Kobayashi**, Y. Ura, S. Kimura, J. Sugiyama

Section B
Loews New Orleans Hotel
St. Landry

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Rafael Luque
Cosponsored by ENVR and I&EC
S.O. Obare, *Organizer, Presiding*
G. Beckham, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 144. Continuous manufacturing of fine chemicals for a sustainable future. **C. Kappe**

8:30 CELL 145. Glucose to fructose isomerization over natural MgO catalysts. **K. Triantafyllidis**, A. Marianou, C. Michailof, S. Karakoulia, E. Iliopoulou, A. Lappas

8:55 CELL 146. Catalytic transfer hydrogenolysis of aromatic ethers promoted by the bimetallic Pd/Ni system. E. Paone, R. Pietropaolo, **F. Mauriello**, R. Luque

9:20 CELL 147. Nanoparticle mediated conversion of biorenewables into biofuels and commodity chemicals. **S.O. Obare**

9:45 Intermission.

10:00 CELL 148. Biological conversion of thermochemical wastewater streams. **G. Beckham**

10:25 CELL 149. Polysaccharides dissolution in deep eutectic solvents (DES) a promising approach for biomass refining. E. Morais, M. Freire, C. Freire, J. Coutinho, **A. Silvestre**

10:50 CELL 150. Catalytic C-O bond cleavage in non-derivatized alcohols. **J.S. Samec**

11:15 CELL 151. Benign-by-design methodologies for a more sustainable future: from nanomaterials to heterogeneous (photo)catalysis and biomass conversion. **R. Luque**

Section C
Loews New Orleans Hotel
St. Tammany

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Cosponsored by AGFD, ANYL and CARB
H. Kamitakahara, C. Wong, *Organizers*
K.J. Edgar, T.J. Heinze, L.L. Kiessling, L. Wang, *Presiding*

8:05 CELL 152. End-functionalization of polysaccharide in cellulose chemistry. **H. Kamitakahara**, R. Suhara, M. Yamagami, H. Kawano, R. Okanishi, K. Miki, T. Asahi, A. Yoshinaga, Y. Tanaka, T. Takano

8:30 CELL 153. Multivalent glycopolypeptide-based micelles and polymersomes. **S. Lecommandoux**

8:55 CELL 154. Microbial polysaccharides in pathogens. **L.L. Kiessling**

9:20 CELL 155. Automated glycan assembly as basis for material science. **P.H. Seeberger**

9:45 Intermission.

10:00 CELL 156. Streamlining complex carbohydrate synthesis through enzymatic procedures. **G. Boons**

‡*Cooperative Cosponsorship*

10:25 CELL 157. Phase 2 clinical results of a carbohydrate (GloboH)-based cancer vaccine. **C. Yu**

10:50 CELL 158. Influenza vaccine and ADCC. **C. Ma**, C. Wong

11:15 CELL 159. Siglecs: Putting the brakes on the immune system. **J.C. Paulson**, B. Arlian, S. Duan, L. Edgar, C. Kikuchi, M. Macauley, C. Nycholat, L. Pang, A. Srivastava

Section D
Loews New Orleans Hotel
Beauregard

Assembly & Colloidal Interactions of Cellulose Nanocrystals
Cosponsored by COLL
Financially supported by EPNOE
C. Schütz, *Organizer*
W. Thielemans, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 160. Water inclusion-based modeling of CNC film assemblies through non-contact dielectric characterization. **C.D. Emiroglu**, B. Natarajan, J. Obrzut, J.W. Gilman

8:30 CELL 161. Fabrication technique for clearly transparent nanopaper from highly concentrated cellulose nanofiber dispersion. **T. Kasuga**, N. Isobe, H. Koga, M. Nogi

8:55 CELL 162. Formation of flexible hybrid materials with embedded hierarchically structured components. **B.L. Tardy**, B.D. Mattos, L. Garcia Greca, K. Klockars, M. Borghei, O. Rojas

9:20 CELL 163. Novel multilayered nanostructured drug delivery systems obtained by layer-by-layer assembly of cellulose nanocrystals. M. Maia, C. Vilela, R.J. Pinto, B. Valente, T. Carvalho, **C. Freire**

9:45 Intermission.

10:00 CELL 164. Kinetic of polymers and nanoparticles adsorption on cellulose nanocrystal surfaces. Z. Jaafar, C. Mauroy, A. Villares, A. Brosse, J. Vigourox, N. Beury, C. Levard, J. Rose, M. Lahaye, **B. Cathala**

10:25 CELL 165. Investigating the interaction of cellulose with lipid membranes. **Y. Navon**, B.R. Jean, L. Heux

10:50 CELL 166. Self-Assembling crustacean-mimetic CNC/polymer nanocomposites with hierarchical energy dissipation mechanisms. **A. Walther**

11:15 CELL 167. Buckling-based metrology for measuring the Young's modulus of polyvinyl alcohol – cellulose nanocrystals thin biocomposites layers. **J. Desmaisons**, E. Niinivara, U. Gill, A. Dufresne, E.D. Cranston, **J. Bras**

Section E
Loews New Orleans Hotel
Terrebonne

Wood-Based Materials for Energy & Water

Wood-Based & Related Materials

Cosponsored by ENFL, ENVR and MPPG
L. Hu, S. Lee, Z. Ren, L. Wagberg, J. Zhu, *Organizers*
L. Nyholm, *Organizer, Presiding*
H. Zhu, *Presiding*

8:05 CELL 168. Functional bacterial cellulose for energy and biomedical application. **G. Yang**

8:30 CELL 169. Chitin nanofiber transparent paper: A renewable material platform for green electronics and energy devices. **J. Jin**

8:55 CELL 170. Hierarchical alignment of chitin fiber as a novel non-woven separator for metal-based batteries. J. Jin, **S. Kang**

9:20 CELL 171. The use of the layer-by-layer technology and low density networks of cellulose nanofibrils for preparing new materials for energy storage. **L. Wagberg**, M. Hamedi, A. Marais, G. Nystrom, H. Francon, H. Granberg, J. Erlandsson

9:45 Intermission.

10:00 CELL 172. Advanced wood nanostructures for solar water. **L. Hu**

10:25 CELL 173. Form factor-free, flexible paper power sources. **S. Lee**

10:50 CELL 174. Optimum utilization ways of cellulose toward high-power, environmentally friendly, and renewable energy storage devices. **H. Yu**

11:15 CELL 175. Solar-driven simultaneous steam production and electricity generation from seawater. **J. Zhou**

11:40 Concluding Remarks.

MONDAY AFTERNOON

Section A
Loews New Orleans Hotel
LaFourche/Pointe Coupee

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Cosponsored by BIOL, BIOT and POLY
U.P. Agarwal, R.H. Atalla, H. Chanzy, A. Isogai, *Organizers*
T. Kondo, T. Larsson, *Presiding*

1:00 Introductory Remarks.

1:05 CELL 176. Elucidation of hemicelluloses functions on lignification using artificial wood cell wall based on honeycomb-patterned cellulose. **Y. Uraki**

1:30 CELL 177. Optimal pretreatment of lignocellulosic biomass for better biorefinery. **Y. Horikawa**

1:55 CELL 178. Hydrogen disorder: the nature of crystalline cellulose. **P. Chen**

2:20 CELL 179. Enzymes degrading cellulose: From molecular mechanisms to traffic simulator. **K. Igarashi**

2:45 CELL 180. Highly strong materials constructed from cellulose solution based on formation of nanofibers. **L. Zhang**, A. Lyu, J. Cai, C. Chang, K. Zhu, D. Ye

3:10 CELL 181. Natural nanofiber films welding via ionic liquids. **G. Reyes**, O.J. Rojas, M. Borghei

Section B
Loews New Orleans Hotel
St. Landry

Lignin: From Fundamentals to New Materials & Applications

Fundamental Understanding of Lignin

Cosponsored by ENVR and POLY
C. Crestini, H. Lange, M. Mattinen, M. Sipponen, *Organizers*
M.K. Osterberg, *Organizer, Presiding*
S. Sarkanen, *Presiding*

1:00 Introductory Remarks.

1:05 CELL 182. Probing the mechanical effects of lignification on primary cell walls. **S.N. Kiemle**, D. Cosgrove

1:30 CELL 183. Molecular dynamics simulation study of interaction of lignin monomers and dimers with lipid bilayers. **X. Tong**, B. Novak, D. Moldovan

1:55 CELL 184. Density functional theory study of cross-coupling of lignin with tricin and ferulates. **T.J. Elder**, L. Berstis, G. Beckham, M.F. Crowley

2:20 CELL 185. Novel structural model for softwood kraft lignins. **C. Crestini**, H. Lange, M. Sette, D. Argyropoulos

2:45 CELL 186. The chemical character of lignin: Interactions with solvents. **L. Petridis**

3:10 CELL 187. Green gasoline and road diesel from black liquor in three steps. **J.S. Samec**

3:35 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

Frontiers in Glycoscience, Bridging the Gap Between Carbohydrate & Polysaccharide Chemistries
Cosponsored by AGFD, ANYL and CARB
H. Kamitakahara, C. Wong, *Organizers, Presiding*

1:05 CELL 188. Dissolution of cellulose in NaOH/zinc nitrate at low temperature. **A. Lyu**, S. Wang, L. Zhang

1:30 CELL 189. Highly selective polysaccharide modification. B.L. Nichols, Y. Dong, L.I. Mosquera-Giraldo, L. Taylor, **K.J. Edgar**

1:55 CELL 190. Withdrawn

2:20 CELL 191. Amphiphilic polysaccharide Schiff base delivery vehicles for controlled release of biologically active compounds. **B.L. Nichols**, K.J. Edgar

2:45 CELL 192. Chemical modifications of nano/cellulose for functional materials. **K. Zhang**

3:10 CELL 193. Scalable, continuous process to ethyl cellulose-based oleogels. **R. Appell**, D. Malotky

3:35 Concluding Remarks.

Section D
Loews New Orleans Hotel
Beauregard

Assembly & Colloidal Interactions of Cellulose Nanocrystals
Cosponsored by COLL
Financially supported by EPNOE
C. Schütz, *Organizer*
W. Thielemans, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL 194. Exploring cellulose nanocrystal dispersion dynamics: A Landau-de Gennes approach. **M. Pospisil**, M.J. Green, V.A. Davis, M. Noor, P. Saha, S. Abdulquddos

1:30 CELL 195. Tunability of water/cellulose nanocrystal interactions through altered hydrolysis conditions and subsequent purification. **E. Niinivaara**, C. Fraschini, J. Bouchard, E.D. Cranston

1:55 CELL 196. Surface charge influence on the chemistry, colloidal stability, and self-assembly of cellulose nanocrystals. **T. Abitbol**, H.S. Marway, A.F. Palermo, S.A. Kedzior, X. Yang, A. Franey, D.G. Gray, J. Moran-Mirabal, E.D. Cranston

2:20 CELL 197. Grafting well-defined CO_2-responsive polymers *to* cellulose nanocrystals via nitroxide-mediated polymerization: Effect of graft density and molecular weight on dispersion behaviour. J. Glasing, J. Bouchard, P. Champagne, P.G. Jessop, **M.F. Cunningham**

2:45 CELL 198. Pickering emulsions stabilized by esterified cellulose nanocrystals: application to the elaboration of polymer latexes and colloidosomes. **G. Sebe**, A. Werner, V. Héroguez, Z. Zhang

3:10 CELL 199. Incorporating cellulose nanocrystals into the core of polymer latex particles through polymer grafting. **S.A. Kedzior**, M. Kiriakou, E. Niinivaara, M.A. Dubé, C. Fraschini, R.M. Berry, E.D. Cranston

Section E
Loews New Orleans Hotel
Terrebonne

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Value Added from Agricultural Crops

Cosponsored by AGFD, ENFL, ENVR and MPPG
B. Ghotra, L.A. Lucia, T. Younos, *Organizers*
A. Ayoub, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL 200. Value-added and sustainable product processing of by-products from agricultural commodities — with grape as the main model. **C. Xu**, X. Xie, J. Lu, M.R. Marshall

1:30 CELL 201. Advances in immobilized enzyme systems to mine value-added products from agricultural waste streams. **J.M. Goddard**

1:55 CELL 202. Value added applications of peanut processing plant waste. **L.L. Oehrl**, B.J. Hess

2:20 CELL 203. Structural evaluation during conversion stages of lignin feedstocks to carbonaceous products. **D.P. Harper**

2:45 CELL 204. Catalytic upgrading of bio-oils derived from agricultural crop residue: A study of application and mechanism. **N. Hao**, A. Ragauskas, Y. He, S. Laursen

3:10 CELL 205. Comparison of biodiesel crude glycerol pretreatments of bamboo for efficient enzymatic hydrolysis. **L. Ji**, J. Jianxin

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards:

‡*Cooperative Cosponsorship*

Symposium in honor of Fengqi You
Sponsored by I&EC, Cosponsored by CELL

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
M. Roman, *Organizer*
8:00–10:00

40, 48, 51, 70, 81, 83, 85-86, 88-89, 95-97, 101-103, 107-108, 111-112, 115-117, 120-125, 128, 131-134, 191, 204. See previous listings.

230, 283, 322, 327, 384, 392, 399, 413. See subsequent listings.

TUESDAY MORNING

Section A
Loews New Orleans Hotel
LaFourche/Pointe Coupee

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Cosponsored by BIOL, BIOT and POLY
U.P. Agarwal, R.H. Atalla, H. Chanzy, A. Isogai, *Organizers*
S.H. Kim, T. Rosenau, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 206. Branched structures of cellulose molecules in high-molecular-mass fraction of softwood revealed by SEC/MALLS/IR/UV analysis. **A. Isogai**, Y. Ono, T. Saito

8:30 CELL 207. Temperature and strain induced frequency shifts of infrared signals of cellulosic materials: Fundamental and applied aspects. **C. Altaner**, F. Guo

8:55 CELL 208. Xyloglucan-cellulose organization in plant primary cell walls: Reassessment by imaging approaches. Y. Zheng, X. Wang, Y. Chen, E. Wagner, **D. Cosgrove**

9:20 CELL 209. The state of cellulose in cold alkali solutions. **T. Larsson**

9:45 Intermission.

10:00 CELL 210. Nanoporous celluloses: Previously unknown forms, as the best primary feedstocks for energy, chemical and agricultural feed production. **R.H. Atalla**, R. Atalla

10:25 CELL 211. Cell wall carbohydrate structure and biosynthesis in pathogenic oomycetes
. **V. Bulone**

10:50 CELL 212. Investigating individual wood cell wall layers with X-ray micro and nano beams. **M. Mueller**

11:15 CELL 213. Transformations of wood-cellulose ultrastructure: Investigations of molecular-conformation, extent of disorder, and crystallinity by FT-Raman spectroscopy. **U.P. Agarwal**

Section B
Loews New Orleans Hotel
St. Landry

Lignin: From Fundamentals to New Materials & Applications

Advances in Lignin Characterization
Cosponsored by ENVR and POLY
M. Mattinen, M.K. Osterberg, M. Sipponen, *Organizers*
C. Crestini, H. Lange, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 214. Evaluation of lignin branching. **E.A. Capanema**, M. Balakshin

8:30 CELL 215. New insights into the molecular structure of kraft lignin and its mechanisms of formation. C. Lancefield, H.L. Wienk, R. Boelens, B. Weckhuysen, **P. Bruijnincx**

8:55 CELL 216. Lignomics: Nanoscience, structure determination and MW-based fractionation using SEC, MS, STEM, TD-pyr-GC/MS and thermal carbon analysis. **A. Kubatova**, A. Andrianova, S. Lu, S. Reagen, J.E. Schumaker, H. Bilek, I.P. Smoliakova, E. Kozliak

9:20 CELL 217. Characterization of protein amino acid residues and a monolignol conjugate in whole plant cell walls by solution-state 2D NMR and their interference with authentic *p*-hydroxyphenyl (H) unit estimation. **H. Kim**, D. Padmakshan, Y. Li, J. Rencoret, S. Karlen, R.D. Hatfield, J. Ralph

9:45 Intermission.

10:00 CELL 218. Structural characterization of corn stover lignins after combinatorial pretreatment strategies. **S. Shinde**, Z. Liu, M.L. Olson, X. Wang, N. Hao, C. Yoo, S. Bhagia, J. Dunlap, Y. Pu, K. Kao, M. Jin, J. Yuan, A. Ragauskas

10:25 CELL 219. Study of a new chemical derivatization method on lignin hydroxyl groups for size exclusion chromatography analysis. **E. Esakkimuthu**, M. Brochier-Salon, N. Marlin, G. Mortha

10:50 CELL 220. Structural analysis of lignin isolated from a novel biorefinery process and identification of condensed structures using 2D NMR. **L. Lagerquist**, P. Eklund

11:15 CELL 221. Do lignin-carbohydrates complexes (LCC) survive to acid chlorite delignification? **D. Da Silva Perez**, M. Gonzalez Martinez, C. Dupont, X. Meyer, C. Gourdon, C. Crestini

11:40 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Ning Yan
Cosponsored by ENVR and I&EC
J. Zhang, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 222. Carbohydrate stabilization with formaldehyde prevents degradation and facilitates sugar recovery during biomass depolymerization. **J. Luterbacher**

8:30 CELL 223. Withdrawn

8:55 CELL 224. Highly efficient molecular transformation using ordered alloys as catalysts. **S. Furukawa**

9:20 CELL 225. Exploiting support effects and composition in Cu based bimetallic catalysts for sustainable chemical conversion. **P. Christopher**

9:45 Intermission.

10:00 CELL 226. Perovskite catalysts for oxidative coupling of methane. Y. Sim, J. Yoo, D. Kwon, **J. Jung**

10:25 CELL 227. Halide perovskite nanostructures for energy harvesting and optoelectronics. **L. Dou**

10:50 CELL 228. Techno-economic and life cycle optimization of multiple waste-to-energy and resources pathways. H. Yang, **X. Wang**

11:15 CELL 229. Shell biorefinery: Dream or reality? **N. Yan**

Section D
Loews New Orleans Hotel
Terrebonne

Biobased Water Purification System Approaches
Cosponsored by AGFD, CHAS and ENVR
H. Jameel, N.S. Simon, *Organizers*
R. Gonzalez, L.A. Lucia, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 230. Dynamics and kinetics of marine exoskeleton-based heavy metal biosorption and desorption. **C. Londono Zuluaga**, H. Jameel, L.A. Lucia, R. Gonzalez

8:30 CELL 231. Chitosan derivatives for metal removal from wastewater. **S. Mincke**, T. Grima, I. Verheye, G. Du Laing, C.V. Stevens

8:55 CELL 232. Polymer-grafted chitosan for applications in dye and heavy metal removal and recovery from water. O. Garcia-Valdez, E. Madill, B. Tsai, M. Cunningham, **P. Champagne**

9:20 CELL 233. Modified cellulose ethers aerogels for the removal of organic pollutants from wastewater. **D. Petri**

9:45 Intermission.

10:00 CELL 234. Hydrophobization by polymer adsorption to bacterial cellulose structures. **P. Spiliopoulos**, A. Lokka, E. Kontturi

10:25 CELL 235. Biosorbent films based on nanocellulose and lysozyme nanofibers for efficient removal of mercury (II) from natural waters. N.H. Silva, P. Figueira, C. Vilela, R.J. Pinto, I. Marrucho, M.E. Periera, **C. Freire**

10:50 CELL 236. Nanopaper nanofiltration membranes from seawater suspensions of TEMPO-CNF. **A. Mautner**, K. Lee, A. Bismarck

11:15 CELL 237. Nanocellulose for use in enhanced oil recovery: Transportation of nanocellulose dispersions through porous media. **E. Heggset**, R. Aadland, C. Dziuba, K. Syverud, O. Torsæter, S. Bryant

Section E
Loews New Orleans Hotel
Beauregard

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Food, Water & Energy from Sustainable Crops
Cosponsored by AGFD, ENFL, ENVR and MPPG
B. Ghotra, L.A. Lucia, T. Younos, *Organizers*
A. Ayoub, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 238. Sustainable production of foods with berry polyphenols. **B.W. Bolling**

8:30 CELL 239. Food processing alters phytochemicals and their absorption. **J. Cooperstone**

8:55 CELL 240. Withdrawn

9:20 CELL 241. Realizing integrated supercritical fluid biorefineries for the green processing of grains and oilseeds. **O. Ciftci**

9:45 Intermission.

10:00 CELL 242. How the commercialization of novel peppermint varieties is contributing to sustainable production of peppermint oil. **M. Morris**, D. Holmgren, J. Liu, J.G. Zeevaart, M. Bubniak

10:25 CELL 243. Microalgae cultivation for wastewater treatment and bioenergy production. **A. Bhatnagar**, E. Daneshvar

10:50 CELL 244.
Value-added bio-based food products. **M.P. Yadav**

11:15 CELL 245. Investigation of sugar beets as a feedstock for sustainable alternative jet fuel in south Florida. **C. Dorado**, R.G. Cameron, K. Cooper

TUESDAY AFTERNOON

Section A
Loews New Orleans Hotel
LaFourche/Pointe Coupee

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Cosponsored by BIOL, BIOT and POLY
R.H. Atalla, H. Chanzy, A. Isogai, *Organizers*
U.P. Agarwal, *Organizer, Presiding*
Y. Nishiyama, *Presiding*

1:00 Introductory Remarks.

1:05 CELL 246. Junji Sugiyama and CERMAV: A long lasting impact. **H.D. Chanzy**

1:30 CELL 247. Allomorphic transition in native cellulose promoted by ultrasounds. **K. Mazeau**, P. Chen, Y. Ogawa, L. Heux, S. Molina Boisseau, J. Putaux, Y. Nishiyama

1:55 CELL 248. Ultrastructural characterization of cellulosics by solid state NMR: has everything been done? **L. Heux**

2:20 CELL 249. Mutation analysis to explore potential functional differences among plant CESA isoforms
. **C.H. Haigler**, J.N. Burris

2:45 CELL 250. All-atom structural model of plant cellulose synthase and cellulose synthase complex. A. Singh, **Y.G. Yingling**

3:10 CELL 251. Diffraction studies of cotton fibers. **A.D. French**

3:35 Intermission.

‡*Cooperative Cosponsorship*

4:00 CELL 252. An electron crystallographer of cellulose microfibrils–revisit and hereafter. **J. Sugiyama**

Section B
Loews New Orleans Hotel
St. Landry

Lignin: From Fundamentals to New Materials & Applications

Lignin Valorization in Biorefineries

Cosponsored by ENVR and POLY
C. Crestini, H. Lange, M. Mattinen, M.K. Osterberg, M. Sipponen, *Organizers*
C. Crestini, D. Da Silva Perez, *Presiding*

1:00 Introductory Remarks.

1:05 CELL 253. Improving lignin homogeneity by aqueous solvent fractionation. **A. Jääskeläinen**, T. Liitiä, T. Tamminen

1:30 CELL 254. Zambezi biorefinery: A novel lignin source with unique properties. **A.L. Jongerius**, J.C. Van der Waal, G. Van Klink, E. Dejong

1:55 CELL 255. Lignin acidolysis during thermomechanical wood refining. **M. Tasooji**, C.E. Frazier

2:20 CELL 256. Role of dispersion and polar interactions in the adsorption of cellulases onto lignin. **M. Roman**, F. Jiang, C. Qian, A. Esker

2:45 CELL 257. Fractionation of sugar cane bagasse lignin using hydrotropic process. **P.E. Fardim**

3:10 CELL 258. Influence of fractionation and phenolation of Lignoboost – Kraft-lignin on formation and properties of lignin-hydrogels. **A. Hoffmann**, M. Bremer, U. Fischer, J.P. Nong, S. Fischer

3:35 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

Functional Structures from Wood-Based Materials

Fibers & Filaments

Cosponsored by COLL
Financially supported by Adolphe Merkle Institute, University of Fribourg, MDPI Fibers
E. Filpponen, T. Nypelo, J.O. Zoppe, *Organizers*
M.K. Ek, S. Spirk, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CELL 259. Characterization of the quality of pulp fines and their effect on paper properties. M. Mayr, R. Eckhart, A. Thaller, **W. Bauer**

1:30 CELL 260. Wood-based cellulosic fibers: Current challenges and further developments from an industrial perspective. **M. Pichler**, C. Bisjak, C. Sperger, J. Innerlohinger

1:55 CELL 261. Effect of particle dispersion on mechanical properties of filaments made of cellulose nanofibrils. **K. Haakansson**

2:20 CELL 262. Developing Pd-based nanomagnets in the lignocellulose matrix for natural fiber welding applications. **D.P. Durkin**, J.R. Morey, K.J. Livi, P.C. Trulove, H. ElBidweihy

2:45 CELL 263. Interfacial interactions in lignin /carbon nanotubes precursors of carbon fibers. **M.G. Laborie**, J. Badorreck, G. Sivasankarapillai, M. Walter

3:10 CELL 264. Characterization of composite fibers from wood-based polymers: Investigation as a carbon fiber precursor. **D. Sawada**, H. Zahra, M. Trogen, H. Sixta, N. Byrne, M. Hummel

Section D
Loews New Orleans Hotel
Terrebonne

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Cosponsored by ENVR and POLY
J. Campos-Teran, O. Rojas, *Organizers*
M.L. Auad, *Organizer, Presiding*

1:00 Introductory Remarks .

1:05 CELL 265. Lignin and nanocelluloses in food and other emulsions. S. Huan, L. Bai, B.L. Tardy, M. Ago, J. Lehtonen, **O.J. Rojas**

1:30 CELL 266. Applications of molten salt hydrates in fractionation, conversion, and valorization of lignocellulosic biomass. **X. Pan**

1:55 CELL 267. Withdrawn

2:20 CELL 268. Depolymerized lignin & acrylate-based renewable photopolymers. **K. Rajan**, J.K. Mann, Y.N. Regmi, D.P. Harper, N. Labbé, S.C. Chmely

2:45 CELL 269. What method to measure natural fiber size distribution in polymer composite? Advantages and limitations of 2D scanner, automated analysis and microtomography. E. Di Giuseppe, R. Castellani, S. Dobosz, J. Malvestio, F. Berzin, J. Beaugrand, C. Delisée, B. Vergnes, S. Hamdi, **T. Budtova**

3:10 CELL 270. Carbon fibers from nanofibrillated lignocellulose for supercapacitors. **L. Wang**, M. Borghei, P. Lahtinen, A. Papageorgiou, M. Lundahl, M. Ago, O. Rojas

Section E
Loews New Orleans Hotel
Beauregard

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Biomaterials Processing

Cosponsored by AGFD, ENFL, ENVR and MPPG
B. Ghotra, L.A. Lucia, T. Younos, *Organizers*
A. Ayoub, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL 271. Modification of the cellulosic surfaces through adsorption of reactive polysaccharides. A. Bouchut, A. Pettignano, C. Moreau, B. Cathala, M. Lecourt, M. Petit-Conil, J. Bernard, A. Charlot, **E. Fleury**

1:30 CELL 272. Microalgae: A new resource for processing bio-based polymer materials. **N. Le Moigne**, F. Delrue, J. Sassi, G. Arrachart

1:55 CELL 273. Synthesis and characterization of hemicellulose-based hydrogels. **J. Pawlak**, W. Geng, R.A. Venditti

2:20 CELL 274. Application of subcritical water to the sustainable production of agricultural crops and processing by-products. **J.W. King**, L. Howard, K. Srinivas

2:45 CELL 275. Ionic liquids: New Generation of additives for biopolymers processing. **S. Livi**

3:10 CELL 276. Towards added value biomaterials: Hemicellulose isolation and its application as thermoreversible network. **W. Farhat**, R.A. Venditti, A. Ayoub, M. Taha, N. Mignard, F. Becquart

WEDNESDAY MORNING

Section A
Loews New Orleans Hotel
Lafourche

Plant Heteropolysaccharides: Interactions within Lignocellulosics, New Modifications & Future Applications

Structures, Interactions, & Extraction of Plant Heteropolysaccharides

Cosponsored by CARB
K.S. Mikkonen, *Organizer*
M. Tenkanen, F. Vilaplana, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 277. Non-cellulose wood polysaccharides – a need for a stricter structural and functional classification? **G. Henriksson**, J. Berglund, J. Wohlert, M. Lawoko, S. Aminzadeh, M.E. Lindström, F. Vilaplana

8:30 CELL 278. Nanostructures, molecular interactions, and anisotropic elastic moduli of lignocellulosic cell walls with moisture. **N. Rahbar**, J. Jakes

9:20 CELL 279. Chromatographic fractionation of lignocellulosic extracts: Influence of the extraction conditions. **P. Pontalier**, V. Oriez, J. Peydecastaing

9:45 Intermission.

10:00 CELL 280. Influence of the molecular structure of wood hemicelluloses on the recalcitrance of lignocellulosic biomass. A. Martínez-Abad, A. Jimenez Quero, J. Berglund, N. Giummarella, G. Henriksson, M.E. Lindström, J. Wohlert, M. Lawoko, **F. Vilaplana**

10:25 CELL 281. Withdrawn

10:50 CELL 282. Extraction and characterization of residual hemicellulose in dissolving pulp. C. Kim, J. Lee, T. Treasure, J. Skotty, T. Floyd, S.S. Kelley, **S. Park**

11:15 CELL 283. Structural colour from a helicoidal cellulose fibres architecture in the cell wall of *Margaritaria nobilis*. **L.M. Steiner**, Y. Ogawa, M. Busse-Wicher, P. Dupree, S. Vignolini

Section B
Loews New Orleans Hotel
St. Landry

Lignin: From Fundamentals to New Materials & Applications

Nanoscaled Materials from Lignin

Cosponsored by ENVR and POLY
C. Crestini, M. Mattinen, M. Sipponen, *Organizers*
H. Lange, M.K. Osterberg, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CELL 284. Fabrication of lignin nanoparticles for developing natural broad-spectrum sunscreens. **Y. Qian**, J. Wang, D. Yang, X. Ouyang, X. Qiu

8:30 CELL 285. Colloidal lignin particles towards gluing biological matrices. **M. Mattinen**, M.K. Osterberg

8:55 CELL 286. Lignin-based nanocarriers for the controlled release of agrochemicals. **D. Yiamsawas**, W. Kangwansupamonkon, M. Prawatborisut, D. Crespy

9:20 CELL 287. Producing lignin nanoparticles directly from raw lignocelluloses at ≤ 80 °C in an aqueous system using a recyclable acid hydrotrope. **J. Zhu**

9:45 Intermission.

10:00 CELL 288. All-lignin approach for preparation of cationic colloidal lignin particles and their use in Pickering emulsions. M. Sipponen, T. Leskinen, **M.K. Osterberg**

10:25 CELL 289. Facile fabrication of enhanced electrode materials for energy storage using composite of self-assembled lignosulfonate nanosheets and graphene. **W. Meng**, F. Xu, X. Zhang

10:50 CELL 290. Spherical lignin particles for triggered release of anti-inflammatory drugs. **M. Sipponen**, H. Lange, C. Crestini

11:15 CELL 291. Lignin-modified carbon nanotubes/graphene hybrid as efficient flame retardant. **K. Song**, I. Ganguly, I. Eastin, A. Dichiara

11:40 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

Functional Structures from Wood-Based Materials

Paper & Fibrils

Cosponsored by COLL
Financially supported by Adolphe Merkle Institute, University of Fribourg, MDPI Fibers
M.K. Ek, E. Filpponen, S. Spirk, J.O. Zoppe, *Organizers*
T. Nypelo, *Organizer, Presiding*
W. Bauer, *Presiding*

8:05 CELL 292. Novel polysaccharides for strength improvement and coatings for paper and paperboard structures. **J. Fisher**

8:30 CELL 293. Comparing approaches to very high wet adhesion between wet cellulose surfaces. **E. Gustafsson**, D. Yang, R.H. Pelton

8:55 CELL 294. Liquid flame spray (LFS) deposited nanoparticles on natural fibre based substrates for antimicrobial activity. **J. Saarinen**, B.K. Jocelyn, J. Haapanen, M. Gunnell, E. Eerola, P. Huovinen, J. Mäkelä

9:20 CELL 295. Tailored nano-latexes for modification of nanocelluloses: Compatibilizing and plasticizing effects. **J. Engstrom**, F. Hatton, A. Boujemaoui, C. Cobo Sanchez, L. Wagberg, F. D'Agosto, M. Lansalot, L. Fogelstrom, E.E. Malmstrom, A.E. Carlmark

‡*Cooperative Cosponsorship*

9:45 Intermission.

10:00 CELL 296. Industrially relevant cationic starches: Interaction with cellulose thin films. K. Niegelhell, A. Chemelli, T. Griesser, H. Reiter, U. Hirn, **S. Spirk**

10:25 CELL 297. Flow-assisted organization of nanostructured bio-based materials. **N. Mittal**, F. Lundell, L. Wagberg, M. Hedhammar, D. Soderberg

10:50 CELL 298. Morphological and thermal characterization of polysaccharides/protein biocomposites as a function of alcohol and peroxide content. **D. Salas-de la Cruz**, D. Verrill, J. Stanton

11:15 CELL 299. Maintenance of functional effectivity of modified cellulosic fibers during textile refining. **F. Wendler**, M. Krieg, K. Stauche, F. Meister

Section D
Loews New Orleans Hotel
Terrebonne

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Cosponsored by ENVR and POLY
M.L. Auad, O. Rojas, *Organizers*
J. Campos-Teran, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 300. Preparation and properties of solution cast films from pennycress protein isolate. **G.W. Selling**, M. Hojilla-Evangelista, W. Hay, K. Utt, G. Gross

8:30 CELL 301. Encapsulation of valuable algae-based compounds in biopolymeric nanoparticles. S. Ortiz, L. Rodas, S. García-Pérez, R. Parra-Saldívar, J. Campos-Teran, **I. Arroyo-Maya**

8:55 CELL 302. Thermodynamics of algal growth substrates made from renewable macromolecules. **Z. Karimi**, J.M. Passantino, D.W. Herring, G. Proano Pena, D. Blersch, V.A. Davis

9:20 CELL 303. Zinc-free synthetic isoprene rubber vulcanizates using wheat protein as an activator. **B.L. DeButts**, R. Thompson, J.R. Barone

9:45 Intermission.

10:00 CELL 304. Crystallization of polypropylene in the presence of plant tissue. **P.R. Navard**, J. Girones, L. Vo, J. Haudin, L. Freire, V. Song, S. Boyer, C. Barron

10:25 CELL 305. Invasive plants in Western Europe as renewable raw materials for biorefining: The case study of Japanese knotweed. **A. Hospied**, Q. Schmetz, A. Richel

10:50 CELL 306. Utilization of aqueous phase of biomass pyrolysis for synthesis of novel olefins and polyolefins. **M. Barde**, K. Avery, C.W. Edmunds, N. Labbé, M.L. Auad

11:15 CELL 307. Wood biorefinerie In subcritical water conditions. **P. Pontalier**, G. Vilarem, N. Beaufils, L. Rigal, L. Candy

Section E
Loews New Orleans Hotel
Beauregard

Biobased Gels & Porous Materials

Functionalised Nanocellulose Gels

Cosponsored by COLL and PMSE
Financially supported by EPNOE
T. Budtova, *Organizer*
F. Liebner, *Organizer, Presiding*
S.J. Eichhorn, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 308. Structure-property relationship of nanocellulose gels. **L. Mendoza**, W. Batchelor, G. Garnier

8:30 CELL 309. Novel preparation method of self-sustaining hydrogel using only cellulose nanofiber dispersion. **S. Suenaga**, M. Osada

8:55 CELL 310. Tuning rheological properties of polysaccharide gels using hydrophobic cellulose nanocrystals. R. Nigmatullin, J. Scott, K.J. Edler, Y.Z. Khimyak, J. Angulo, **S.J. Eichhorn**

9:20 CELL 311. Dynamic networks of cellulose nanofibrils as a platform for tunable hydrogels, aerogels, and chemical modifications. **T. Benselfelt**, L. Wagberg

9:45 Intermission.

10:00 CELL 312. Sorghum protein based biocomposites reinforced by cellulose nanowhiskers: Effect of hydrolysis time. **W. Li**, B. Mu, Y. Yang

10:25 CELL 313. Cellulose-based gel beads for quantifying the swelling behavior of plant fibers. **P. Karlsson**, T. Larsson, L. Wagberg

10:50 CELL 314. 3D printing functional nanocellulose hydrogels. O. Fourmann, **G. Siqueira**, M. Hausmann, M. Schubert, T. Zimmermann

11:15 CELL 315. Nanostructured hydrogels for potential application in 3-D bioprinting. N.H. Silva, C. Vilela, R.J. Pinto, **C. Freire**

Bioenergy & Bio-Based Chemicals
Sponsored by ENFL, Cosponsored by CELL

WEDNESDAY AFTERNOON

Section A
Loews New Orleans Hotel
Lafourche

Plant Heteropolysaccharides: Interactions within Lignocellulosics, New Modifications & Future Applications

Modification & Future Applications of Plant Heteropolysaccharides

Cosponsored by CARB
M. Tenkanen, F. Vilaplana, *Organizers*
K.S. Mikkonen, *Organizer, Presiding*
U. Edlund, *Presiding*

1:05 CELL 316. Safety considerations of softwood galactoglucomannans in food use. L. Pitkanen, M. Heinonen, **K.S. Mikkonen**

1:30 CELL 317. Extraction of distinct populations of bioactive arabinoxylans from wheat bran using sequential chemo-enzymatic processes. **A. Jimenez Quero**, R. Rudjito, A. Martínez-Abad, A. Ruthes, F. Vilaplana

1:55 CELL 318. Spruce galatoglucomannan stabilized emulsions are potential carriers for bioactive compounds. **H. Zhao**, K.S. Mikkonen, A. Lampi, P. Kilpeläinen, M. Lehtonen

2:20 CELL 319. Enzymatic modification of corn bran arabinoxylan alters the *in vitro* fecal fermentation profiles by human gut microbiota. **X. Zhang**, B. Hamaker

2:45 Intermission.

3:00 CELL 320. Bioplastics and composites from plant heteropolysaccharides. A. Svärd, M. Sterner, **U. Edlund**

3:25 CELL 321. Xylan nanotiles. **A.M. Johnson**, M. Karaaslan, S. Renneckar, S. Mansfield, F. Unda

3:50 CELL 322. Insights into hemicellulose-cellulose interactions from thermochemical pretreatment of model composite materials. **R. Shah**, D. Sawada, B. Evans, S. Pingali, B.H. Davison, H.M. O'Neill

4:15 CELL 323. Solubility and adsorption of different xyloglucan fractions to model surfaces. **S. Kishani**, J. Wohlert, F. Vilaplana, L. Wagberg

4:40 Concluding Remarks.

Section B
Loews New Orleans Hotel
St. Landry

Lignin: From Fundamentals to New Materials & Applications

Carbon Fibers & Chemicals from Lignin

Cosponsored by ENVR and POLY
C. Crestini, H. Lange, M. Mattinen, M.K. Osterberg, *Organizers*
M. Sipponen, *Organizer, Presiding*
D. Argyropoulos, *Presiding*

1:00 Introductory Remarks.

1:05 CELL 324. Against all odds: Carbon nanofibers from unmodified low molecular weight lignin fractions. R. Ebrahimi Majdar, **H. Lange**, F. Basoli, M. Trombetta, C. Crestini

1:30 CELL 325. Ultralight nanofibrous lignin aerogels with outstanding shape-recovery properties. **M. Cho**, M. Karaaslan, H. Wang, S. Renneckar

1:55 CELL 326. Carbon fibers made from cellulose-lignin hybrid filaments. **M. Hummel**, M. Trogen, D. Sawada, H. Sixta, N. Byrne

2:20 CELL 327. Dry-jet wet-spun lignin-based carbon fibre precursors: Phenomena and properties. **J. Bengtsson**, K. Jedvert, T. Köhnke, H. Theliander

2:45 Intermission.

3:00 CELL 328. Electrochemical conversion of Kraft-lignin to valuable products. **S.R. Waldvogel**, M. Zirbes

3:25 CELL 329. Lignin degradation using recyclable formate ionic liquids and microwave. **J. Dai**, A. Patti, K. Saito

3:50 CELL 330. Elucidation of the behavior of lignin in switchable solvents: Partitioning, dissolution and/or self-assembly? **T. Berchem**, T. Lepage, A. Richel

4:15 CELL 331. Aerobic vanadium catalysis for lignin valorization: A bottom-up approach. **G. Licini**

4:40 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

Functional Structures from Wood-Based Materials

Films & Low-Density Composites

Cosponsored by COLL
Financially supported by Adolphe Merkle Institute, University of Fribourg, MDPI Fibers
M.K. Ek, E. Filpponen, T. Nypelo, S. Spirk, *Organizers*
J.O. Zoppe, *Organizer, Presiding*
I. Filpponen, *Presiding*

1:05 CELL 332. Ultrasounds welding of nanocellulosic materials: A proof of concept. C. Monot, B. Harthong, R. Peyroux, D. Imbault, D. Guerin, J. Viguie, **J. Bras**

1:30 CELL 333. Cellulose nanopapers from elephant manure. **A. Mautner**, K. Weiland, A. Bismarck

1:55 CELL 334. Thermal and electrical properties of TEMPO-oxidized nanocellulose films with quaternary alkylammonium carboxylates. **M. Shimizu**, R. Kusumi, T. Saito, A. Isogai

2:20 CELL 335. Polysaccharide film as a ductile substrate for gas phase treatment. **T. Nypelo**, H. Amer, J. Konnerth, A. Potthast, T. Rosenau

2:45 Intermission.

3:00 CELL 336. Cellulose xanthate as an aqueous source to generate functional cellulose thin films. **M. Weißl**, K. Niegelhell, D. Reishofer, A. Zankel, S. Spirk

3:25 CELL 337. Understanding and improvement of mechanical properties in plasticized cellulose acetate polymers. **A. Charvet**, D. Long, C. Vergelati

3:50 CELL 338. Novel method for producing formable low-density materials from self-assembled cellulose nanofibrils. **H.S. Françon**, J. Erlandsson, V. López Durán, H. Granberg, L. Wagberg

4:15 CELL 339. Nano-FTIR spectroscopy: Nanoscale resolved infrared spectroscopy of individual CNC fibers and thin films. **T. Gokus**, P. Schäfer

Section D
Loews New Orleans Hotel
Terrebonne

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Cosponsored by ENVR and POLY
M.L. Auad, J. Campos-Teran, O. Rojas, *Organizers*
D. Estenoz, *Presiding*

1:00 Introductory Remarks.

1:05 CELL 340. Withdrawn

1:30 CELL 341. Imparting moisture resistance to transparent nematic *i*-CNF aerogels by $scCO_2$-antisolvent coating of the interior with ultrathin PMMA layers. S. Plappert, S. Quraishi, J. Nedelec, J. Konnerth, H. Rennhofer, H. Lichtenegger, **F. Liebner**

1:55 CELL 342. Formulation and composition effects in phase transitions of emulsions stabilized by cellulose nanofibrils and an ionic surfactant. **S. Huan**, S. Yokota, L. Bai, M. Ago, M. Borghei, T. Kondo, O. Rojas

‡*Cooperative Cosponsorship*

2:20 CELL 343. Cellulose nanofibrils in ice cream: An analysis of its influence in the matrix structure. **J.A. Velasquez**, C. Gomez Hoyos, A.M. Serpa Guerra, P.F. Ganan, L. Duizer, C. Castro Herazo, D. Goff, R. Zuluaga Gallego

2:45 Intermission.

3:00 CELL 344. Use of cellulose nanofibrils as replacement of xanthan gum in water based drilling fluids for Argentina shale. Y.A. Villada Villada, M. Iglesias, N. Casis, M. Peresin, E. Erdmann, **D. Estenoz**

3:25 CELL 345. Nanocellulose from wood residues for water-based polymer reinforcement. **G. Cheng**, B. Via, L. Wei, N. Stark

3:50 CELL 346. Withdrawn

4:15 CELL 347. Environmental benign and salt-free reactive dyeing of cellulose using a cottonseed oil/water system to achieve high dye fixation. **B. Mu**, H. Xu, Y. Yang

Section E
Loews New Orleans Hotel
Beauregard

Biobased Gels & Porous Materials

Cellulose & Non-Cellulose Gels: Synthesis, Properties, Applications

Cosponsored by COLL and PMSE
Financially supported by EPNOE
T. Budtova, F. Liebner, *Organizers*
N. Baccile, C. Freire, *Presiding*

1:05 CELL 348. Functional agarose hydrogels and composite hydrogels. **M. Gericke**, M. Witzler, A. Enkelmann, G. Schneider, M. Schulze, T.J. Heinze

1:30 CELL 349. Multifunctional hyaluronic acid based hydrogel with enzymatically embedded silver/lignin nanoparticles. **S. Pérez Rafael**, K. Ivanova, I. Stefanov, T. Tzanov

1:55 CELL 350. Developing renewable and high strength hydrogels by incorporating lignin. **K. Rajan**, D.P. Harper, T.G. Rials, D. Carrier, N. Labbé, S.C. Chmely

2:20 CELL 351. Hydrogels from self-assembled microbial glycolipids. G. Ben Messaoud, S. Roelants, L. Van Renterghem, **N. Baccile**

2:45 Intermission.

3:00 CELL 352. Controlling the nanomorphology of anisotropic cellulose II aerogels by diffusion-driven gradual molecular self-assembly in a templating solvent. S. Plappert, H. Rennhofer, H. Lichtenegger, **F. Liebner**

3:25 CELL 353. Microstructural dynamics and rheology of flocculated micro/nanofibrillated cellulose suspensions. **E. Facchine**, O.J. Rojas, S. Khan

3:50 CELL 354. Spreading of water in low density nanocellulose networks: From capillaries to specific surface area. **L. Wagberg**, H. Granberg, J. Erlandsson, H. Francon, F. Zou, R. Östmans

4:15 CELL 355. Low-cost and chemically stable quaternary ammonium salts for cellulose homogenisation. **G.J. Partl**, S. Väinämö, J.K. Helminen, D. Rico del Cerro, I.A. Kilpeläinen, A. King

Bioenergy & Bio-Based Chemicals
Sponsored by ENFL, Cosponsored by CELL

THURSDAY MORNING

Section A
Loews New Orleans Hotel
Lafourche

Advances in Bacterial (Nano) Cellulose Research

Bacterial (Nano)Cellulose Formation, Structure & Medical Applications

Cosponsored by ANYL
M. Gama, *Organizer*
D.O. Klemm, T. Rosenau, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 356. From comparative genomics to BNC structural variants production. **K. Kubiak**, M. Ryngajllo, P. Jacek, M. Jedrzejczak-Krzepkowska, S. Bielecki

8:30 CELL 357. Simulations of cellulose synthesis in bacteria suggested a primer-independent mechanism. **H. Yang**, M. Tien, Y.G. Yingling, J.D. Kubicki

8:55 CELL 358. Modification of bacterial nanocellulose – in terms of (bio)molecular aspect and its application. P.P. Rytczak, M. Ryngajllo, I. Cielecka, **S. Bielecki**

9:20 CELL 359. Design of bacterial nanocellulose materials using a novel matrix technology. **D.O. Klemm**, F. Kramer, S. Nietzsche, K. Petzold-Welcke, T. Richter

9:45 Intermission.

10:00 CELL 360. Withdrawn

10:25 CELL 361. Novel multilayered drug delivery systems based on bacterial nanocellulose for skin treatment. **C. Freire**, C. Vilela, C. Rodrigues, D. Fonseca, A. Silvestre

10:50 CELL 362. Epicite – A new advanced wound dressing made from bacterial cellulose. **D. Kralisch**, N. Hessler, M. Funk, F. Schubert

11:15 CELL 363. Biocellulosis as scaffold for tissue regeneration in modern surgery. **F. Rauchfuss**

Section B
Loews New Orleans Hotel
St. Landry

Lignin: From Fundamentals to New Materials & Applications

Polymers & Resins from Lignin

Cosponsored by ENVR and POLY
C. Crestini, M. Mattinen, M.K. Osterberg, M. Sipponen, *Organizers*
H. Lange, *Organizer, Presiding*
U.P. Agarwal, *Presiding*

8:00 Introductory Remarks.

8:05 CELL 364. Lignin based 3D-printing materials: Printability and performance. **N.A. Nguyen**, S.H. Barnes, K. Meek, C.C. Bowland, J.K. Keum, A.K. Naskar

8:30 CELL 365. Organosolv lignin as epoxy polymer reinforcing agent. R. Kokoli, D. Giliopoulos, P. Lazaridis, A. Fotopoulos, K. Karagiannidis, X. Pappa, **K. Triantafyllidis**

8:55 CELL 366. Novel biobased epoxy resins from depolymerized native lignin. **D. van de Pas**, E. Feghali, K. Torr

9:20 CELL 367. Lignin-caused performance improvements of poly(lactic acid)/CNCs composites. L. Wei, **U.P. Agarwal**, L. Matuana, R. Sabo, N. Stark

9:45 Intermission.

10:00 CELL 368. Prospects for high levels of industrial Kraft lignin (Indulin AT) in functional polymeric materials. Y. Chen, **S. Sarkanen**

10:25 CELL 369. A retrosynthesis perspective on new thermoset resin applications based on industrial Kraft lignin. **M. Jawerth**, M.K. Johansson, S. Lundmark, C. Gioia, M. Lawoko

10:50 CELL 370. Beat it! Foam templated macroporous lignin foams. M. Jalalian, Q. Jiang, **A. Bismarck**

11:15 CELL 371. Elucidation of the phenolated lignin structures and phenolation mechanism. **X. Jiang**, J. Liu, H. Chang, H. Jameel

11:40 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

Functional Structures from Wood-Based Materials

Biosensing & Biomaterials

Cosponsored by COLL
Financially supported by Adolphe Merkle Institute, University of Fribourg, MDPI Fibers
M.K. Ek, E. Filpponen, T. Nypelo, S. Spirk, J.O. Zoppe, *Organizers*
I. Filpponen, M. Laborie, *Presiding*

8:05 CELL 372. Cellulose nanocrystal (CNC) microelectromechanical systems (MEMS) for biosensing. P. Saha, R. Ashurst, **V.A. Davis**

8:30 CELL 373. Derivatization and processing of biodegradable polymers into biomaterials. T. Mohan, T. Maver, M. Kurečič, R. Kargl, T. Elschner, T.J. Heinze, **K. Stana Kleinschek**

8:55 CELL 374. Polymer analogous reactions comparing polysaccharides with polyvinylalcohols. A. Bratuša, K. Stana Kleinschek, **R. Kargl**

9:20 CELL 375. 3D printing wood – a biomimetic approach. **K. Markstedt**, P. Gatenholm

9:45 Intermission.

10:00 CELL 376. Cellulose nanocrystals for fabricating biomimetic cartilage. A. Kumar, K. Lee, H. Liang, **A. Asadi**

10:25 CELL 377. Cellulose nanofibrils from wood as a new substrate for covalent immobilization of pro-drug molecule by click chemistry. **H. Durand**, E. Zeno, I. Baussanne, M. Demeunynck, S. Fort, N. Belgacem, J. Bras

10:50 CELL 378. Acquiring antibacterial and hemostatic properties for polypropylene nonwovens via layer-by-layer surface modification using soybean protein. **A.M. Abdelgawad**, C. Fritz, O.J. Rojas

11:15 CELL 379. Construction of chitosan/rectorite/cellulose nanofibers composites and their applications in biomedical materials. **Y. Du**, A. Lyu, H. Gao, X. Shi

Section D
Loews New Orleans Hotel
Terrebonne

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Cosponsored by ENVR and POLY
M.L. Auad, J. Campos-Teran, *Organizers*
O. Rojas, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL 380. Hybrid nanocelluloses to design functional emulsions. **I. Capron**, J. Mougel, O. Chauvet, B. Cathala, P. Bertoncini, N. Shandilya

8:30 CELL 381. Nanocellulose derivatives: A comparative study of nanocelluloses from wood- and vegetable-based raw materials. **N. Pahimanolis**, J. McKee, H. Mertaniemi, A. Laukkanen

8:55 CELL 382. Control of Pickering emulsion properties by the structural characteristics of nanocelluloses. **C. Jimenez Saelices**, I. Capron

9:20 CELL 383. Continuous filaments from cellulose with impressive wet strength. **A. Tripathi**, M. Ago, **S. Khan**, O. Rojas

9:45 Intermission.

10:00 CELL 384. Sustainable bio-ethanol production from crystalline cellulose promoted by Pd/Fe_3O_4 catalyst. **B. Gumina**, F. Mauriello, C. Espro, R. Pietropaolo, S. Galvagno

10:25 CELL 385. Study of biopolymeric hydrogel interactions with photodynamic systems. **D. Gómez-Maldonado**, R. López-Simeon, A. Topete Camacho, **J. Campos-Teran**

10:50 CELL 386. Cellulose surface modification using polysaccharide multifunctional systems. **I. Vega Erramuspe**, M. Peresin, T.J. Heinze, P.E. Fardim

11:15 CELL 387. Stabilization of cellulose nanocrystal-based Pickering emulsion induced by cellulose nanofibrils: Impact of depletion effect on the phase behavior of emulsion droplets. **L. Bai**, S. Huan, W. Xiang, O. Rojas

Section E
Loews New Orleans Hotel
Beauregard

Biobased Gels & Porous Materials

Biomedical Applications of Polysaccharide Gels & Aerogels

Cosponsored by COLL and PMSE
Financially supported by EPNOE
T. Budtova, F. Liebner, *Organizers*
J. Bras, K. Syverud, *Presiding*

8:05 CELL 388. Cellulose nanofibril hydrogels as scaffolds for tissue engineering. **K. Syverud**, E. Heggset, A. Rashad, K. Mustafa

8:30 CELL 389. Development of nanostructured systems based on poly (3,4-ethylenedioxythiophene) (PEDOT) aerogels of starch/κ-carrageenan for biomedical applications. **R. Zamora**

8:55 CELL 390. Bioinspired capsules based on nanocellulose, xyloglucan and pectin for biomedical applications. **T.**

‡*Cooperative Cosponsorship*

Paulraj, A.J. Svagan

9:20 CELL 391. Biocompatible bacterial cellulose/Ti_3C_2-MXene electroactive composite hydrogels for skin tissue repair and regeneration. **L. Mao**, Z. Shi, G. Yang

9:45 Intermission.

10:00 CELL 392. Green porous Chitosan microspheres as microcarriers for "real" 3D culture of hepatocytes. **L. Huang**, L. Xiao, G. Yang

10:25 CELL 393. Injectable anisotropic cellulose nanocrystal hydrogels as a platform for functional tissue engineering applications. **K.J. De France**, K. Yager, K. Chan, B. Corbett, E.D. Cranston, T. Hoare

10:50 CELL 394. Nanocellulose based materials in liquid for stem cell growth monitoring. **J. Bras**, M. Smyth, C. Picart, J. Foster

11:15 CELL 395. Hemocompatibility of porous sulfonated *Cladophora* cellulose beads towards a blood purification material with anticoagulant properties. **I. Rocha**, N. Ferraz, A. Mihranyan, M. Strömme, J. Lindh

THURSDAY AFTERNOON

Section A
Loews New Orleans Hotel
Lafourche

Advances in Bacterial (Nano) Cellulose Research

Pharmaceutical, Medical & Technical Applications

Cosponsored by ANYL
D.O. Klemm, T. Rosenau, *Organizers*
S. Bielecki, M. Gama, *Presiding*

1:05 CELL 396. Surface microstructured bacterial nano-cellulose for anti-adhesive and anti-fibrotic protection of medical devices. **A. Ferrari**, S. Bottan, F. Robotti, G. Pellegrini, D. Poulikakos, C. Starck

1:30 CELL 397. Bacterial nanocellulose: A natural biopolymer for controlled drug delivery. **D. Fischer**

1:55 CELL 398. Nanocelluloses from cotton waste, bacterial nanocellulose and glycidyl methacrylate grafting: specific adsorption properties towards target molecules. **E. Vismara**, C. Bongio, G. Torri

2:20 CELL 399. Bacterial cellulose 3D structuring towards new applications. **L. Garcia Greca**, J. Lehtonen, B.L. Tardy, J. Guo, O. Rojas

2:45 Intermission.

3:00 CELL 400. Fabrication and evaluation of nanofibrous biomaterials for biomedical applications. **L. Fu**, G. Yang, W. Wan, C. Panchal

3:25 CELL 401. Mechanical response of multi-layer bacterial cellulose nanopaper-reinforced polylactide laminated composites. **M. Hervy**, K. Lee

3:50 CELL 402. Fracture resistance of bacterial cellulose-reinforced poly(methyl methacrylate) composites. **A. Santmarti**, M. Hervy, K. Lee

4:15 CELL 403. (Ultra-)low grammage bacterial cellulose nanopaper-reinforced polylactide composite laminates. M. Hervy, F. Bock, **K. Lee**

4:40 Concluding Remarks.

Section B
Loews New Orleans Hotel
St. Landry

Lignin: From Fundamentals to New Materials & Applications

Biochemical Modification of Lignin

Cosponsored by ENVR and POLY
C. Crestini, H. Lange, M. Sipponen, *Organizers*
M. Mattinen, M.K. Osterberg, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 CELL 404. Enzymatic lignin modification without solvents in water-soluble alkaline conditions. **M.W. Heikkila**, **K. Birikh**, **T. Gronroos**

1:30 CELL 405. Lignin-rich residues originated from a range of pretreatments: Structural characterization and anaerobic microbial biomethane production. **D. Mulat**, J. Dibdiakova, M. Opedal, S. Horn

1:55 CELL 406. Laccase treatment as means to improve membrane filterability of lignin-containing birch hot water extract. **A.K. Kalliola**, T. Tamminen, J. Lahti, T. Virtanen, M. Kallioinen, H. Lange, C. Crestini

2:20 CELL 407. Enzymatic modification of lignin by fungal laccases. **A.S. Meyer**, M. Kabel, L. Munk

2:45 Intermission.

3:00 CELL 408. Towards more uniform technical lignin. **L. Liu**, N. Sathitsuksanoh, M. Cho, S. Chowdhury, S. Renneckar

3:25 CELL 409. Carbon fibers derived from fractionated-solvated lignin. J. Jin, J. Ding, A. Klett, M.C. Thies, **A.A. Ogale**

3:50 CELL 410. Expanding capability of ^{13}C NMR spectroscopy in comprehensive lignin analysis. **M. Balakshin**, E.A. Capanema

4:15 CELL 411. Fungal growth and enzyme production on alkali lignin from grasses. **M. Daou**, D. Navarro, S. Raouche, **C. Faulds**

4:40 Concluding Remarks.

Section C
Loews New Orleans Hotel
St. Tammany

Functional Structures from Wood-Based Materials

Designed Structures & Processing

Cosponsored by COLL
Financially supported by Adolphe Merkle Institute, University of Fribourg, MDPI Fibers
E. Filpponen, T. Nypelo, S. Spirk, *Organizers*
M.K. Ek, J.O. Zoppe, *Organizers, Presiding*

1:05 CELL 412. Ductile and thermoplastic cellulose with novel application and design opportunities. **P.A. Larsson**, E. Linvill, G. Lo Re, S. Östlund, L. Wagberg

1:30 CELL 413. Enhanced functional properties of co-exfoliated graphene doped microfibrillated cellulose composites. **J. Phiri**, L. Johansson, P. Gane, T.C. Maloney

1:55 CELL 414. Bio-based fire retardant and its application in cellulose-based thermal insulation materials. **C. Zheng**, D. Li, M.K. Ek

2:20 CELL 415. Application of nanocotton and nanocollagen on cotton/polyester blend fabric using layer-by-layer (LBL) technique. **S.M. Mansour**

2:45 Intermission.

3:00 CELL 416. From vapour to gas: Optimising cellulose degradation with gaseous HCl. **T. Pääkkönen**, E. Kontturi

3:25 CELL 417. Withdrawn

3:50 CELL 418. Stabilization kinectics of polyacrylonitrile/cellulose nanocrystals composite fibers. **H. Chang**, J. Luo, H.C. Liu, S. Kumar

4:15 CELL 419. Polymer nanocomposites with cellulose nanocrystals: Effects of polymer grafting and processing methods on thermomechanical properties. S. Wohlhauser, J. Natterodt, **J.O. Zoppe**, C. Weder

4:40 Concluding Remarks.

Section D
Loews New Orleans Hotel
Terrebonne

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Cosponsored by ENVR and POLY
M.L. Auad, J. Campos-Teran, O. Rojas, *Organizers*
I. Vega Erramuspe, *Presiding*

1:00 Introductory Remarks.

1:05 CELL 420. Processing of chicken feathers using a deep eutectic solvent. **E. Nuutinen**, A. Jääskeläinen

1:30 CELL 421. Composites from natural resources: Hemp fiber reinforced composites from 3D orthogonal woven preforms and their potential applications in US. **A. Gupta**

1:55 CELL 422. Two-step process for recovery of copper naphthenate from end-of-life railroad ties. **H.L. Haber**, P. Kim, S.C. Chmely, J. Lloyd, Y.N. Regmi, N. Abdoulmoumine, N. Labbé

2:20 CELL 423. Economic analysis of integrated continuous process for colloidal lignin particle via aerosol flow method. **M. Ago**, C. Abbati de Assis, L. Garcia Greca, R. Gonzalez, O. Rojas

2:45 Intermission.

3:00 CELL 424. Synthesis of UV curable poly (ethylene glycol) diacrylate macromere based semi-IPN hydrogel with polysaccharides. **P. Joshi**, S. Breaux, M. Auad

3:25 CELL 425. Incorporation of dialdehyde cellulose microfibrils within a biobased polyfurfuryl alcohol thermosetting matrix: Structure and properties relations. **R. Ganfoud**, N. Guigo, L. Heux, N. Sbirrazzuoli

3:50 CELL 426. Fabrication of strong nanocomposite films with renewable forestry waste/montmorillonite/reduction of graphene oxide for fire retardant. **G. Chen**, F. Peng, C. Yao, R. Sun

4:15 CELL 427. Cross-linkable hydrogels for 3D bioprinting. **N. Alizadeh**, R. Broughton, M. Auad

Section E
Loews New Orleans Hotel
Beauregard

Biobased Gels & Porous Materials

Polysaccharide Foams, Cryogels & Aerogels

Cosponsored by COLL and PMSE
Financially supported by EPNOE
F. Liebner, *Organizer*
T. Budtova, *Organizer, Presiding*
P.E. Fardim, *Presiding*

1:05 CELL 428. Thermal conductivity of bio-aerogels. **T. Budtova**

1:30 CELL 429. Withdrawn

1:55 CELL 430. High porosity cellulose-based foams by ice-templating. C. Antonini, O. Nylén, **T. Geiger**

2:20 CELL 431. On the mechanism of freeze-induced crosslinking of aerogels made from periodate-oxidised cellulose nanofibrils. **T. Pettersson**, J. Erlandsson, P.A. Larsson, L. Wagberg

2:45 Intermission.

3:00 CELL 432. Green synthesis of nanocellulose aerogels decorated with palladium nanoparticles and their application in water purification. **J. Gu**, A. Dichiara

3:25 CELL 433. Cellulose-reinforced and hybrid cellulose-based biofoams for structural and flame resistance applications. **P.E. Fardim**, C. Lange, J. Obradovic

3:50 CELL 434. Cellulose and cellulose composites for carbon dioxide sorption at low and elevated temperatures. R. Dassanayake, C. Gunathilake, A.C. Dassanayake, M. Jaroniec, **N. Abidi**

4:15 CELL 435. Low density foam-formed fibre structures with enhanced elasticity and strength. **K. Torvinen**, T. Pöhler, L. Timo, J. Ketoja

4:40 Concluding Remarks.

CHED

Division of Chemical Education

C. Gauthier, N. Snyder and A. Marsh, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Jani C. Ingram (see ANYL, Tue)

Active Learning in the Undergraduate Analytical Chemistry Curriculum (see *ANYL*, Sun)

Chemical Information Literacy: Innovation, Collaboration & Assessment (see *CINF*, Tue)

Implementing ACS Safety Education Guidelines (see *CHAS*, Mon)

Environmental Chemistry Undergraduate Education in the Classroom, Laboratory & Beyond (see *ENVR*, Mon, Wed)

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10:25 CHED 12. Temperature sensitive paper as a medium to study reaction energies and equilibrium constants. G.G. Via, **R.C. Dudek**

10:45 CHED 13. Optical properties of alloyed noble metal nanoparticles: A nanotechnology experiment for chemistry and engineering students. **T. Vasicek**, S.V. Jenkins

11:05 CHED 14. Thiourea and amidothiourea based rhenium (1) complexes as luminescent and colorimetric anion sensors. **M.O. Odago**

11:25 CHED 15. Science of light and color: A multidisciplinary course for design majors. **L.J. Medhurst**

11:45 CHED 16. Synthesis and Spectroscopic study of a different salicylidene imines as a laboratory exercise. **J.B. Dudek**, J. Bennett

12:05 Concluding Remarks.

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Citizens First!
Cosponsored by CEI
C. Maguire, *Organizer*
R.D. Sheardy, *Organizer, Presiding*
N. Kohan, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 17. Pseudoscience fair crosses chemistry and other disciplines. **F.M. Yarberry**, **J. Schneider**, **S. Turner**

8:55 CHED 18. Fostering a STEM education learning network with community benefits through cooperative partnerships. **L. Robinson**, P.J. Carlson, G. Bishop

9:15 CHED 19. Developing scientific literacy through analysis of news reports. **T. Jordan**, S. Kay, R. DiYanni

9:35 CHED 20. Civic and social responsibility for chemistry majors. **C. Maguire**, N. MirsalehKohan, R.D. Sheardy

9:55 Intermission.

10:20 CHED 21. Maintaining the context-content balance for elementary education students. **B.D. Fahlman**

10:40 CHED 22. Democratized cloud-based computational chemistry in support of undergraduate chemical education and citizen science. **B.B. Magers**, P.J. Carlson, B.D. O'Gwynn, H. McAlexander, D.H. Magers, G. Bishop

11:00 CHED 23. Science in the public interest. **K.K. Oates**

11:20 CHED 24. Assessing citizenship. **S. Carroll**

11:40 Concluding Remarks.

Section D
New Orleans Marriott Convention Center
Blaine Kern B

Strategies Promoting Success of Two-year College Students

T.B. Higgins, *Organizer*
L.J. Anna, A.M. Palmer, *Organizers, Presiding*

Integrating Polymer Science in the Curriculum (see *POLY*, Mon, Tue)

SOCIAL EVENTS:

Chemistry Educators Luncheon, 12:00 PM: Sun

Social Reception, 5:30 PM: Sun

SUNDAY MORNING

Section A
New Orleans Marriott Convention Center
Blaine Kern C/D

Chemistry Teachers Day Program
Cosponsored by SOCED
S.C. Rukes, *Organizer*
K.B. Gosciniak, *Presiding*

8:00 Registration.
8:30 Introductory Remarks.

8:35 CHED 1. Development of organic solar cells. **L. Zhai**

9:05 CHED 2. Beyond Benign solar cell technology: Making dye-sensitized solar cells with blackberries. **K. Anderson**, **M.C. Enright**, **L.J. Doody**

9:40 CHED 3. Energy and safety in high school chemistry labs. **I.G. Cesa**

10:10 Intermission.

10:15 CHED 4. Solution chemistry as an introduction to food science, energy, and water. **S.B. Mitchell**

10:50 CHED 5. Looking at chemical education around the world. **J. Holman**

11:20 CHED 6. How to use AACT demonstrations in a first and second year chemistry class. **J.L. Ball**, **K.B. Gosciniak**, **K. Duncan**

Section B
New Orleans Marriott Convention Center
Blaine Kern A

Using Light, Color & Spectroscopy to Increase Student Engagement in the Laboratory

J. Bennett, *Organizer*
J.B. Dudek, M.O. Odago, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 7. Simple and green synthesis of colorful, fluorescent, photochromic, and thermochromic imines for organic chemistry laboratory. **J. Bennett**

8:55 CHED 8. Thought-provoking colorful sophomore organic chemistry laboratory experiment. **A.B. Waghe**, A.A. Waghe

9:15 CHED 9. Fostering student understanding of spectroscopy in a general chemistry laboratory. **K. Schnitzenbaumer**, J. Snyder, J.L. Brown-McDonald, R.E. Rosenberg

9:35 CHED 10. Understanding fluorescence instrumentation using guided inquiry. **M.P. Hill**, E. Nam

9:55 CHED 11. Discover light, and understand matter. **J. Schmeisser**, **S. Glazier**

10:15 Intermission.

8:30 Introductory Remarks.

8:35 CHED 25. Implementation of the ALEKS chemistry placement test as a tool for student success. **J. Alexander**, A. Wenz

8:55 CHED 26. Developing a mobile-compatible interactive game for naming molecular compounds. **V. Flaris**, J. Ziegler, E. Lehner

9:15 CHED 27. Expanding access to instrumentation through strategic partnerships. **C.J. Stromberg**, K.H. Bennett, D. Ellis, P. Wood, W. Nellis, P. Sheppard, G. Patterson

9:35 Intermission.

9:45 CHED 28. Strategies for overcoming significant challenges faced by the two-year college student. **S. Botha**, **D.M. Lewis**, **R. Wooten-Moyer**, **A.J. Sanders**

10:05 CHED 29. Attachment theory: Guiding STEM majors through significant change. **B.M. Fetterly**

10:25 CHED 30. The right course for the right student. **S. Burchett**, **J.L. Hayes**

10:45 Intermission.

10:55 CHED 31. Trying on teaching: The learning assistant program at a two-year college. **C.P. Schick**

11:15 CHED 32. Exploring the capacity to improve teacher education (ExCITE). C. Benjamin, S. Donnelly, R. Durren, S. Emerson-Stonnell, M.L. Fink, P. Hastings, V. Lewis, **M.C. Rhoten**, L. Shilling

11:35 CHED 33. Bridges to the baccalaureate: A partnership between Baton Rouge Community College and Louisiana State University to promote student success. **S.L. Watt**, G. Thomas, M.G. Miller, S. Guzman, L. Younger, I.M. Warner, G. Ferreyra

11:55 Concluding Remarks.

Section E
New Orleans Marriott Convention Center
Fulton

Research in Chemistry Education

New & Noteworthy

G.T. Rushton, J.P. Walker, *Organizers, Presiding*
R. Komperda, A. Moon, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 34. Graduate student instructors' knowledge for teaching organic chemistry. **G.V. Szymczak**, A. Moon, M. Connor, E. Zotos

9:15 CHED 35. Thinking processes associated with undergraduate chemistry students' success at applying a molecular-level model in a new context. **M.A. Teichert**, **L.T. Tien**, L. Dysleski, **D. Rickey**

9:55 Intermission.

10:10 CHED 36. Students' perceptions of a project-based organic chemistry laboratory environment: A phenomenographic approach. **N. Burrows**, S.R. Mooring

10:50 CHED 37. Differential use of study approaches by students of different achievement levels. **D.M. Bunce**, R. Komperda, M.J. Schroeder, D.K. Dillner, S. Lin, M.A. Teichert, J. Hartman

11:30 Concluding Remarks.

Section F
New Orleans Marriott Convention Center
Blaine Kern E

NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Anasazi Instruments, Bruker BioSpin, JEOL, Magritek, Mestrelab
D.P. Soulsby, A.S. Wallner, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 38. NMR spectra of dietary supplements. **J.T. Ippoliti**, G. Larson

8:55 CHED 39. Using ^{19}F-NMR spectra in organic teaching labs. **M.L. Druelinger**, **D.L. Dillon**, J.P. Hatfield

9:15 CHED 40. Introducing carbon-13 NMR into the initial molecular model building activities of organic chemistry. **S.A. Hershberger**

9:35 Intermission.

9:50 CHED 41. Organic laboratory activities for teaching heteronuclear nmr to undergraduates. **S.M. Schelble**

10:10 CHED 42. Using a multi-step synthesis and progressive paper to teach NMR spectroscopy in a capstone course. **L. Bastin**, S. Van Bramer

10:30 CHED 43. Fractional hybridization e.g. $sp^{2.5}$, exists and is useful for distinguishing close ^{13}C chemical shifts. **D.D. Clarke**

10:50 Concluding Remarks.

Section G
New Orleans Marriott Convention Center
Magnolia

Undergraduate Research Papers

Organic & Medicinal Chemistry

C.V. Gauthier, *Organizer*
J.V. Ruppel, N.L. Snyder, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 44. Synthesis of an ethylene-linked calixarene dicavitand scaffold: Continued development and optimization of synthetic routes. **E. Peterson**, N.A. Yakelis, J. Freeman

8:45 CHED 45. Synthesis of multipodal organic ligand frameworks for use in combining CMPO groups. **B.G. Wackerle**, S.M. Biros

8:55 CHED 46. Diarylpyrolinol silyl ether as organocatalyst for asymmetric cycloaddition of β,β-unsaturated aldehydes to 3-hydroxyoxindoles to produce spirocyclic β-lactones in aqueous media. **K. Mills**, A.D. Headley, B. Ni

9:05 CHED 47. Synthesis of amides using microwaves and titanium dioxide. **E. Peters**, M. Wentzel

9:15 CHED 48. The use of chiral, non-racemic homoallylic amines as building blocks for piperidine synthesis. **H. Allen**, M.G. Donahue

‡*Cooperative Cosponsorship*

9:25 Intermission.

9:35 CHED 49. Scalable synthesis of cancer preventing benzylmorpholines. **J. Torgunrud**, M.M. Bobylev

9:45 CHED 50. 4-dimethylamino chalcone synthesis optimization and medicinal properties. **H. Cox**, J. Alexander

9:55 CHED 51. Progress on the synthesis of carbohydrate porphyrin conjugates for the photodynamic inactivation of mycobacterium tuberculosis. **L. Russell**, M. Burch, D. Dennis, J.V. Ruppel, N.L. Snyder

10:05 CHED 52. Towards the synthesis of bacteriochlorin glycoconjugates. **N. Abualeinan**, M.R. Parris, D. Dennis, M. Burch, N.L. Snyder, J.V. Ruppel

10:15 CHED 53. Synthesis of new novel CK1d inhibitors as potential therapeutics for Alzheimer's disease. **C. Gettridge**, V. Jha, H. Duong, M. Bratton, J. Sridhar

10:25 Intermission.

10:35 CHED 54. Inhibition of lysyl oxidase in breast cancer cells using derivatized β – aminopropionitrile. **K.A. Johnston**, K.M. Lopez

10:45 CHED 55. Antimycobacterial compounds isolated from marine bacteria and their potential role in biofilm formation. **D. Mellor**, J.A. Trischman

10:55 CHED 56. Antimycobacterial compounds from a marine bacterium isolated from the surface of *Ulva californica*. **K. Moorman**, E. Paul, J.A. Trischman

11:05 CHED 57. Identification of a pharmacophore capable of potentiating ß-lactam antibiotics in methicillin-resistant *Staphylococcus aureus* (MRSA) via fragment based screening. **K. Gillard**, M. Seeman, H.B. Miller, M.S. Blackledge

11:25 Concluding Remarks.

Section H
New Orleans Marriott Convention Center
Fleur De Lis

Chemistry Education Research: Graduate Student Research Forum

A. Hjerstedt, J.M. Pratt, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 58. Comparison of emission spectra from various light sources: A physical chemistry education outreach project. **A.E. Steen**, K.D. Scott, N. Hammer

8:55 CHED 59. Theory of planned behavior applied to high school chemistry teachers implementing next generation science standards. **A. Pierce**, C.E. Brown

9:15 CHED 60. Identifying epistemic games to assist in improving students' chemistry reasoning. **S. Couture**, H. Sevian

9:35 CHED 61. Authentic environmental chemistry research in the high school classroom. **N. May**, J.L. Spencer, A. Watson, L. Bricker, R. Dershimer, K.A. Pratt, G.V. Szymczak

9:55 Intermission.

10:10 CHED 62. Transitioning to eBooks: Student use of various textbook features. **E. Day**, N.J. Pienta

10:30 CHED 63. Optimistic student predictions vs. reality in first semester chemistry. **M. Leake**, D. Mlsna

10:50 CHED 64. The long-term and cumulative effect of online metacognitive training in general chemistry. **B. Casselman**, C.H. Atwood

11:10 CHED 65. Integrating scale themed instruction into an undergraduate anatomy and physiology course. **V. Fisher**

11:30 CHED 66. Using analogies as formative assessment tool to help students learn in chemistry. **D.V. Xue**, M.N. Stains

11:50 Concluding Remarks.

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
Blaine Kern C/D

Chemistry Teachers Day Program
Cosponsored by SOCED
S.C. Rukes, *Organizer*
K.B. Gosciniak, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 67. The *Journal of Chemical Education* in the precollege classroom. **D. Cullen**, G.T. Rushton

1:45 CHED 68. Award Address
(James Bryant Conant Award in High School Chemistry Teaching Sponsored by the Journal of Chemical Education and ChemEd X). The chemistry of opportunity: From the commode to the Conant Award. **B.J. Kennedy**

2:15 CHED 69. Demonstrations, experiments and research involving the Diet Coke and Mentos experiment. **T.S. Kuntzleman**

2:55 CHED 70. Serendipity in the history of chemistry. **D.E. Lewis**

3:25 Intermission.

3:30 CHED 71. What's in the water? Modelling, measuring and visualizing solutions. **T.M. Loschiavo**

4:00 CHED 72. Chemical security education in US educational system. **A. Nelson**

4:25 CHED 73. Polymer science and engineering laboratory activities for the high school classroom developed by RET participants at the University of Southern Mississippi. **S.E. Morgan**, K. Wingo, J. Brownlow, J. Sorrell, R. Hooper

5:05 Concluding Remarks.

Section B
New Orleans Marriott Convention Center
Blaine Kern A

Process-Oriented Guided Inquiry Learning (POGIL)

R.S. Moog, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 74. POGIL and The POGIL Project. **R.S. Moog**

1:55 CHED 75. Assessing POGIL process skills in general chemistry using standards-based grading. **J.G. Davis**

2:15 CHED 76. Information processing of POGIL models. **S.G. Prilliman**

2:35 Intermission.

2:45 CHED 77. Incorporating dynamic models into POGIL activities for general chemistry. **S. Gardiner**, J. Johnston

3:05 CHED 78. Providing students an opportunity to learn chemistry: combining interactive lecture demonstrations, computer simulations, and POGIL-ish activities in a large lecture setting. **T.J. Greenbowe**, D.B. Exton, D.R. Sullivan

3:25 CHED 79. Framework to support instruction and assessment of noncovalent interactions in general chemistry and biochemistry. **V.M. Thorsell**, J.A. Loertscher, J.E. Lewis, A.M. Mercer, A. Dragon, J.D. Pagdanganan, M.T. Werth

3:45 Intermission.

3:55 CHED 80. POGIL activity clearinghouse: Helping authors to create, test, and distribute peer-reviewed POGIL activities. **S. Garrett-Roe**, C. Fish, M.P. Garoutte, M.S. Reeves, C.M. Teague, R.M. Whitnell, A. Grushow, S.S. Hunnicutt

4:15 CHED 81. Significance of significant figures: Introducing metrology in freshman chemistry lab. **M. Howard**

4:35 CHED 82. Implementing POGIL in a flipped organic chemistry lecture. J. Lamblin, L. Luckins, **A. Mueller**

4:55 CHED 83. Are two POGIL's better than one? A study done across multiple semesters. **E.L. Bailey**

5:15 Concluding Remarks.

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Citizens First!
Cosponsored by CEI
R.D. Sheardy, *Organizer*
C. Maguire, *Organizer, Presiding*
L. Robinson, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 84. Stewardship of public waterways: Immersion in the Chesapeake Bay environment. **M.C. Rhoten**, M.L. Fink

1:55 CHED 85. Non-majors general chemistry course as a forum to promote civic responsibility. **N.M. Crompton**

2:15 CHED 86. Sharing your research with the general public: A trip to the mall. **N. Mirsaleh-Kohan**

2:35 CHED 87. Teaching green chemistry principles in environmental chemistry. **S.J. Bachofer**

2:55 Intermission.
3:20 Panel Discussion.
4:35 Concluding Remarks.

Section D
New Orleans Marriott Convention Center
Blaine Kern B

Green Chemistry Student Chapters: Stories of Success

M.C. Enright, J. MacKellar, *Organizers, Presiding*

1:30 Introductory Remarks.

1:50 CHED 88. Splashing into green C=chemistry with bath fizzies! **S. Margis**, **S. Turner**, **S. Stokes**, **E.N. Tran**, **J. Schneider**, **C.L. Emmerling**, G.R. Naumiec, F.M. Yarberry

2:00 CHED 89. ACS Green Chemistry Division at UPR-Aguadilla: A story of continuous success. **L. Acevedo-Soto**, **A.E. Hernandez**, B.J. Ramos-Santana, R.A. Estremera-Andújar, C.A. Nieves-Marrero

2:10 CHED 90. Green chemistry at the University of Tennessee at Martin. **M. Kerbersky**, S. Oliva, T. Rinehart, S.E. Max, B. Ide, W.L. Kuenzinger, A.H. Shelton

2:20 Intermission.

2:40 CHED 91. Making a difference: Green chemistry in West Virginia. M. Nicolay, A. Smith, R. Morris, **M.W. Fultz**

2:50 CHED 92. Green chemistry activities at Tennessee Technological University. **R. Baker**, A.J. Carroll

3:00 CHED 93. Raising green chemistry awareness on college campuses and throughout the Toledo community. **C.M. Schreidah**, M.P. Klingberg, E.N. Kenney, G.T. Hymel, M.J. Demmings, E.T. Diemler, J.D. Koffman, O.M. Tharp, J.P. Fife, D.K. Kaeley, N. Mai, E.P. Kippenhan

3:10 Intermission.

3:30 CHED 94. $(gc)^2$: Gordon College's commitment to green chemistry. **Q. Dougherty**, L. Atlas, V. Ganss, A.H. Kjellson, S. Lareau, I.J. Levy

3:40 CHED 95. Innovation for a healthier planet: Green Chemistry student activities at the University of New England. **J. White**, **K.A. Chalmers**, A.E. Keirstead

3:50 CHED 96. ACS UPRB: Emerging as green chemistry ambassadors. **D. Rivera-Rodriguez**, L. Santiago, N.I. Estarellas San Miguel, J. Oyola, B. Padilla Maldonado

4:00 Concluding Remarks.
4:20 Discussion.

Section E
New Orleans Marriott Convention Center
Fulton

Perspectives on Climate Change Literacy & Education: Local to International
Cosponsored by CEI
K.E. Peterman, *Organizer*

‡*Cooperative Cosponsorship*

G.P. Foy, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 97. Climate change: Reasons for hope. **T.J. Watson**

1:55 CHED 98. Climate change and perspective: Local and global views on problems and solutions in climate change. **J. White**, G.P. Foy, K.E. Peterman

2:15 CHED 99. Biology and climate change: The emergence of biofuels. **Z.J. Snier**, K.E. Peterman, G.P. Foy

2:35 CHED 100. Water's role in climate change. **M. Civitella**, G.P. Foy, K.E. Peterman

2:55 Intermission.

3:05 CHED 101. Understanding of climate science among deaf and hard-of-hearing laboratory technology students improve with the ACS Climate Science Toolkit. **A.D. Ross**, T.E. Pagano

3:25 CHED 102. Withdrawn

3:45 CHED 103. Feasability of implementing solar power as a primary source of power. **J. Pothoof**, K.E. Peterman, G.P. Foy

4:05 CHED 104. Innovations of renewable resources and the role of the US at the UNFCCC 23rd Conference of Parties. **H. Kruelle**, G.P. Foy, K.E. Peterman

4:25 Panel Discussion.
4:35 Concluding Remarks.

Section F
New Orleans Marriott Convention Center
Blaine Kern E

NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Anasazi Instruments, Bruker BioSpin, JEOL, Magritek, Mestrelab

D.P. Soulsby, A.S. Wallner, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 105. Nuclear magnetic resonance: The initial student experience in a university/high school collaboration. **E. Gray**, **M.J. Fromerth**

1:55 CHED 106. Incorporation of benchtop NMR spectroscopy into undergraduate laboratory curricula: Challenges and considerations. **S. Riegel**, J. Araneda

2:15 Intermission.

2:30 CHED 107. A multi-outcome experiment for the preparation of enamines in the undergraduate organic chemistry teaching laboratories. **K. Yearty**, R. Maynard, R.C. Moore, R.W. Morrison

2:50 CHED 108. Structure elucidation of an unknown organic molecule using spectroscopic techniques. **J.A. Pigza**

3:10 CHED 109. A multi-outcome experiment involving the green oxidation of alcohols in the undergraduate teaching laboratories. **K. Yearty**, C.E. Glessner, R.W. Morrison

3:30 Concluding Remarks.

Section G
New Orleans Marriott Convention Center
Magnolia

Undergraduate Research Papers

Analytical & Physical Chemistry

C.V. Gauthier, N.L. Snyder, *Organizers*
J.V. Ruppel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 110. Taming SERS headspace sampling with temperature control. **R.H. Thompson**, M.N. Alam, W. Senanayake, D.E. Thompson

1:45 CHED 111. Characterization of thirdhand smoke constituents on aged smoke-exposed fabrics using high resolution mass spectrometry. **H. Bayat**, A. Whitlatch, W. Jiang, Q. Zhang, S.F. Schick, T.B. Nguyen

1:55 CHED 112. Analysis of E-cigarette fluids with direct sample injection (DSI) GC-MS/MS. **K. Rogers**, K.J. Bisceglia, L. Huang

2:05 CHED 113. Identification of 2-butanone and other VOC's in ivy plants exposed to cigarettes. **J.C. Carter**

2:15 CHED 114. SPME-GC/MS analysis of bacterial volatile organic compound biomarkers for ventilator associated pneumonia. **S.E. Worthy**, C.J. Taylor

2:25 Intermission.

2:35 CHED 115. Using 2D J-resolved NMR to understand carbohydrate conformations. **S. Culver**, J.S. Rhoad

2:45 CHED 116. Isothermal titration calorimetry study of the ligand exchange of oleate-CdSe quantum dots with pyridine. **L.P. Hicks**, J.D. Keene

2:55 CHED 117. Adsorption and hydrolysis of volatile methyl siloxanes on alumina surfaces. **K. Fabrizio**, K.M. Stocker

3:05 CHED 118. Using microstructures of gold-coated photodefinable glass as substrates for surface enhanced Raman spectroscopy. K. Tantawi, **Y. Musa**, S. Dowd, R. Kamali, E.A. Waddell, J. Williams

3:15 CHED 119. Far-infrared synchrotron spectroscopy of formic acid. **K. Hull**, P. Raston

3:25 Intermission.

3:35 CHED 120. Using mathematical tools to characterize chromatin geometries in crystal, cryo-EM and simulated structures. **O. Maxian**, S. Todolli, W.A. Olson

3:45 CHED 121. Multicomponent flexible film of organometallic polymers with polyimide as high *k* and low loss dielectric. **C.M. Anastasia**, S. Nasreen, G.M. Treich, M.L. Baczkowski, M. Tefferi, Y. Cao, G. Sotzing

3:55 CHED 122. Amino acid-derived decorporation agents for radionuclides. **B.M. Jones**, A.D. Parfenov, M.Y. Farraj, J.D. Dignam, K.J. Friedrich

4:05 CHED 123. Polyaniline and nickel hexacyanoferrate modified Prussian blue electrochemical sensors. **M. Byrne**, D. Budner

4:15 CHED 124. Designing a Let-7i detection strategy to elucidate disease states. **A. Gee**, J. Grennell, S. Sitaula, M.F. Ali

4:25 Concluding Remarks.

Section H
New Orleans Marriott Convention Center
Fleur De Lis

Chemistry Education Research: Graduate Student Research Forum

A. Hjerstedt, J.M. Pratt, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 125. Acclimation of first-year graduate teaching assistants to the undergraduate organic chemistry instructional laboratories. **K. Yearty**, R.W. Morrison

1:55 CHED 126. Teaching assistants' topic-specific pedagogical content knowledge in ^{1}H NMR spectroscopy. **M. Connor**, G.V. Szymczak

2:15 CHED 127. Creation of an undergraduate certificate in chemistry education program: Updates and findings. **E.L. Atieh**, D.M. York

2:35 CHED 128. Understanding perceptions and beliefs biochemistry instructors hold and the influence these factors have on their personal style of teaching. **F.K. Lang**, G.M. Bodner

2:55 Concluding Remarks.

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

SUNDAY EVENING

Section A
ErnestN. Morial Convention Center
Hall D

General Posters

I.J. Levy, *Organizer*

7:00–9:00

CHED 129. Biennial Conference on Chemical Education: A place to share information about the teaching and learning of chemistry. **J.M. Sophos**, R.S. Cole, J. Henderleiter Aldrich, D.S. Heroux, S.S. Hunnicutt, I.J. Levy, S.R. Mooring, M. Orgill, C. Sorensen-Unruh, D.G. Sykes, V.M. Williamson

CHED 130. Changing the course of chemistry: Adopting the green chemistry commitment. **D. Ward**, A.S. Cannon, I.J. Levy

CHED 131. Participant feedback on laboratory argumentation BCCE workshops: Why do I want to incorporate argumentation into my lab instruction? **M.T. van Opstal**, J.P. Walker, D.I. Del Carlo

CHED 132. Biotechnology NSF S-STEM program at Western Kentucky University. **K. Williams**

CHED 133. STEM academy: A summer program for NSF S-STEM scholars. **R. Montgomery**, P.A. Shelton, M. Gibson, R. Witmer, J. Devito, B. Bradley

CHED 134. Chemical science investigation: Sandia National Laboratories. **J.M. Sears**, T.J. Boyle, B.A. Hernandez-Sanchez, J. Bremmer

CHED 135. Teaching diversity in second-semester organic chemistry: A contemporary, student-centered approach. **J. Gavenonis**

CHED 136. Applied mathematics and aeospace engineering academy for middle school girls. E.A. Nalley, **M.E. Brown**, M. Magness, T. Sullins

CHED 137. 'Blobology' and other chemistry concepts unleashed: Enhancing the undergraduate chemistry curriculum with 3D printing. **S. Ryan**

CHED 138. Investigating the effect of deliberative democracy on students' perceptions of science and confidence interpreting scientific material. **R. Komperda**, K. Hosbein, J. Barbera, E.E. Shortlidge, G.P. Shusterman

CHED 139. ACS meets IUPAC: Chemical nomenclature and the role of NTS. **M.M. Rogers**, **M.A. Strausbaugh**, **D. Rabinovich**

CHED 140. Looking back – looking forward: Analyses of ACS Examinations and the anchoring concepts content maps as tools for evaluating curricula. **S. Srinivasan**, J.J. Reed, K.L. Murphy, T. Holme, J.R. Raker

CHED 141. Design and implementation of chemistry curriculum for fire fighters in Macau. **P.K. Yuen**, C.D. Lau, E.M. Yen

CHED 142. Using the resources available: Faculty recruiting prospective students in STEM. **M.W. Fultz**

CHED 143. Humor in the classroom: Increasing classroom attendance and engagement through humor. **J. Meyer**

CHED 144. Virtual practice in STEM teaching assistant professional development: Using a mixed-reality teaching simulator to enhance classroom discourse in student-centered learning environments. **E. Saitta**

CHED 145. Comparing the productivity of science-specific and general databases for chemistry primary literature searches. H. Schlarman, **S.D. Wiediger**

CHED 146. Impact of curricular and non-curricular research involvement in STEM persistence. **M. Bolanos**, A.M. Ruiz, B.L. Gonzalez

‡*Cooperative Cosponsorship*

CHED 147. Withdrawn

CHED 148. Liquid nitrogen ice cream: College student conceptual chemistry understanding and intended goals for chemistry outreach events. **J.M. Pratt**, E.J. Yezierski

CHED 149. Using a scanning electron microscope as an outreach education tool. **B.J. Bellott**

CHED 150. Meeting our students where they are: Using text messaging to both promote effective studying and provide formative assessment in introductory chemistry. **D.G. Herrington**, **P.L. Daubenmire**, **R. Sweeder**, **M. Smith**, **E. Stumpe**

CHED 151. Using Instagram as a tool to help undergraduate students in chemistry. **A.J. Roering**, S.C. Silver, J. Mondloch, A.L. Korich

CHED 152. Taking a step toward the future: Being a learning assistant at a two-year college. **C.P. Schick**, A. Tariq, V.L. Miller

CHED 153. Sci-phi: An honors seminar on the science and philosophy of *Dr. Who*. **S.E. Hubbard**, M.K. Douglass

CHED 154. Using humor as an attention focusing tool in a liberal arts chemistry class. **B. Budy**

CHED 155. CHEM 115 – A new model for under-prepared chemistry students. **G. Smeureanu**, D.M. McGregor, P. Mills

CHED 156. Chemistry of fashion: Course for nonscience majors. **K.A. Tallman**

CHED 157. Teaching chemoinformatics at the undegraduate level. **J.L. Medina-Franco**, F. Saldívar-González

CHED 158. From KDD to computational toxicology: A course for graduate students in Mexico. **K. Martinez Mayorga**, K. Gonzalez-Ponce

CHED 159. Conceptual understanding of the linear least-squares expressions by means of mechanical analogs. **D.A. Engebretson**, J. Carey

CHED 160. PhET simulations assigned transparently in introductory chemistry. **K.A. Kaiser**, D. Nguyen-Graff, L. Ye

CHED 161. Remote interview methods. **J.M. Trate**, C.J. Luxford, M.A. Teichert, J.L. Schneider, K.L. Murphy

CHED 162. Integrating writing and computing in the general chemistry curriculum. **S. Bidwell**, **H. Harb**, H.P. Hratchian, M. Colvin, E.J. Menke, P. Gibbons, A. Zanzucchi, J. Leslie

CHED 163. Compute-to-Learn: Authentic learning via development of interactive computer demonstrations within a peer-led studio environment. M. Jafari, A.R. Welden, K. Williams, B. Winograd, **E. Mulvihill**, H.P. Hendrickson, M. Lenard, A.C. Gottfried, E. Geva

CHED 164. Research to practice: Examining the application of a construct map in support of biochemistry students' understanding of the physical basis of interactions. **S. Feola**, **A.M. Mercer**, P. Lemons, V.M. Thorsell, J.A. Loertscher, J.E. Lewis

CHED 165. Development of an inventory to measure students' understandings of quantization and probability using representations of the electronic structure of the atom. **Z. Allred**, S. Bretz

CHED 166. Are they the same or not the same? Close-ended versus open-ended assessments for student learning in chemistry. **L. Ye**

CHED 167. Development of a concept inventory to assess students' understandings of enthalpy and entropy changes in the context of dissolving and precipitation. **T.N. Abell**, S. Bretz

CHED 168. Investigating students' conceptions of chemical kinetics and reaction coordinate diagrams. **M. Croisant**, S. Bretz

CHED 169. Task complexity measures and Item response theory parameters: How are they related? **T.C. Pentecost**, J.R. Raker, K.L. Murphy

CHED 170. Effects of undergraduate student perceptions of inquiry-based laboratory experiences on future research interests. **D.M. Oldendorf**, T. Gupta

CHED 171. Enhancing the teaching ability of young teachers relying on the construction of the course team. **Z. Wang**, Z. Jiang

CHED 172. Development of assessments for student understanding of core chemistry ideas in introductory biology. **A.T. Kararo**, R. Matz, K. Parent, A. Gotwals, S.M. Underwood

CHED 173. Active learning assessment in a Biochemistry course. **C.E. Brown**, R.M. Hyslop

CHED 174. Standards based grading in the chemistry classroom: Assessing outcomes, making grading simple and maintaining rigor. **S.A. Toledo**

CHED 175. Assessing the effect of empirical reasoning support on student learning outcomes in general chemistry. A. Rod, R. Friedkin, D. Weiman, **J.S. Alexander**

CHED 176. Influence of test blueprint publication on student perceptions and performance in an inorganic chemistry course. **K. Young**, S. Lashley, S. Murray

CHED 177. Climate change science: Measuring ancient temperatures and atmosphere compositions. **P.R. Robinson**

CHED 178. Paper spectrometers: The intersection of environmental chemistry and engineering. **A. Kahl**

CHED 179. NanoEarth: An earth and environmental nanotechnolgy collaborative for research, education, outreach, and diversity. **M. Chan**, T. Pruiitt, P.J. Vikesland, M.F. Hochella

CHED 180. Chemical entrepreneurship in a typical chemical instrumental analysis course. **P.J. Carlson**, L. Robinson, G. Bishop

CHED 181. Investigation of nucleation mechanisms in the candy-cola soda geyser. **T.S. Kuntzleman**, B.T. Shadley, M. Nydegger, N. Doctor, D.J. Campbell

CHED 182. Contextualizing general chemistry with biological applications: How collaborative learning and problem-solving supports may help. R.A. Garner, J.M. Maguire, K.A. Leamy, J.R. Miller, L.E. Ritchey, **P.C. Bevilacqua**

CHED 183. Investigation of student attitudes and understanding in an online versus traditional introduction to inorganic chemistry course. **H. Nennig**, L. Salzer, R.M. Theisen

CHED 184. Interteaching in the general chemistry classroom: A low-tech alternative to the conventional "flipped" approach. **K.J. Feierabend**, B.T. Karazsia

CHED 185. Simulation use in general chemistry: Improving student conceptual understanding. **R.D. Sweeder**, J.R. Vandenplas, D.G. Herrington

CHED 186. Withdrawn

CHED 187. An integrated laboratory-based and guided inquiry approach to teaching the second semester of the general chemistry sequence. **T.L. Longin**, D.B. Wacks, D.L. Van Engelen

CHED 188. Implementation and assessment of a successful one-semester general chemistry that replaces the traditional full-year sequence. **W. Kennerly**, K. Frederick, K. Sheppard

CHED 189. Analysis of general chemistry lecture discourse regarding gases and its effect on students' perception of chemical representations. **M.L. Head**, A. Gallimore, I. Brozino, J. Sukumar, K. Forsberg

CHED 190. Encouraging general chemistry students to come to office hours. **D.B. King**

CHED 191. General chemistry performance expectations: Report on a workshop and the nucleation of a community. **D.J. Wink**, A. Donovan

CHED 192. NanoExplorers: A high school summer science academy A STEM enrichment activity. E.A. Nalley, **M. Magness**, M.E. Brown, B. Schmidt, D. Coffee, J. Drake

CHED 193. Roadmap to success: Connecting urban high school students with Syracuse University research experience. B. Kunnath, G. Bonomo, **M.M. Gillett-Kunnath**, K. Ruhlandt-Senge

CHED 194. Determination of ethanol concentration using Raman spectroscopy. **S. Meyer**, **E. Marshall**, K.H. Bennett, S.M. Ensel, C.J. Stromberg

CHED 195. ZnO nanocrystals imaged with scanning electron microscopy: An interdisciplinary undergraduate laboratory module. **J.M. Fritsch**, J.C. Mann

CHED 196. Pre-laboratory instruction: An investigation of effectiveness by mode of delivery. **L. Aronne**, A. George, C. Nagle, J. Styers, A. Combs

CHED 197. Active learning does not stop in lecture: Carry over into the general chemistry lab setting. **A. Jameer**, **A. Sower**, R.L. Falconer, A. Caster

CHED 198. Molecular dipole moments & solvent polarity: Concepts bridging molecular and bulk-matter phenomena in physical chemistry instruction. **P.O. Sandusky**

CHED 199. Nitric acid as a weak acid: Interpreting evidence from Raman spectroscopy. **E.M. Rezler**, J.E. Haky, A.C. Terentis, S. Hyvarinen

CHED 200. Identification of chemical signatures from latent fingerpritns using a Griffon 450 GCMS. **K. Jankowski**

CHED 201. POGIL activity linking thermodynamic parameters of protein unfolding to structure using differential scanning fluorimetry data in the biophysical chemistry classroom. **P. Emery**, E.J. Yezierski, R.C. Page

CHED 202. Surface tension, density, and refractive index of binary water: Monoalcohols liquid systems. **H. Bascal**

CHED 203. Determining enantiomeric excess in ibuprofen. **A. Frangiadis**, G.P. Foy

CHED 204. Distilling the rainbow: A simple distillation for the sophomore organic chemistry lab. P. McKegg, **J. Patrone**

CHED 205. Organic chemistry students' challenges with making connections between reactions and reaction coordinate diagrams. **M. Popova**, S. Bretz

CHED 206. Big fish in a big pond: Tools and techniques to make a large organic chemistry class feel like a small one. **A.E. Keirstead**

CHED 207. Integration of iPads into the organic chemistry sequence. **B.A. Provencher**, J. Franco

CHED 208. Hybrid teaching & beyond: Use of videos across the organic chemistry curriculum. **R.L. Woodward**, C.S. Reid

CHED 209. Labeled mechanism arrows in organic chemistry. **J. Mullins**

CHED 210. Modification of a classic acid-neutral separation experiment for a first semester organic chemistry lab. **T.J. Brunker**, K.P. Reber

CHED 211. OrganicERs: A cCWCS community of organic chemistry educators. J. Houseknecht, **A. Leontyev**, V.M. Maloney, J.L. Muzyka, R.D. Rossi, C. Welder, **L. Winfield**

CHED 212. Using molecular polygons to characterize effects of geometry on macrocycle self-assembly in the organic teaching laboratory. **A. Schafer**, E.J. Yezierski, C. Hartley

CHED 213. Microwave-assisted isolation of eugenol from cloves. **K.R. Overly**

CHED 214. Course based undergraduate research in the organic chemistry laboratory. **M. Hunsen**

CHED 215. Change is inevitable: A perspective on the evolving instruction of first year organic chemistry. **M.L. Druelinger**, **A.M. Schoffstall**

CHED 216. Factors influencing the retention of concepts between first and second semesters of organic chemistry. **W.E. Brenzovich**, W. Hollis

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CHED 217. Grignard reactions using unknown aldehydes or ketones. **D.C. Haagenson**

CHED 218. Synthesis and analysis of merocyanine dye: A wet/dry lab approach in undergraduate organic chemistry laboratory. **A.A. Waghe**, **A.B. Waghe**

CHED 219. Concept of effective mass in understanding quantum confinement in quantum dots and nanocrystals. **D.A. Engebretson**, R.M. Bercaw

CHED 220. Modernization of traditional physical chemistry experiments. **A.S. Frantzen**

CHED 221. Does supplemental instruction inprove grade percentages in organic chemistry. **J.A. Jenson**, R. Claus

MONDAY MORNING

Section A
New Orleans Marriott Convention Center
Blaine Kern C

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry

M.H. Towns, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 222. Herding cats: Chemical education scholarship at a "compass" school. **D.I. Del Carlo**

8:55 CHED 223. Relationship between student study time, satisfaction and exam grade in two chemistry courses. **J.R. Pribyl**, M. Hadley, S. Bowman

9:15 CHED 224. Everything old is new again: A story of finding a disseration relevant many years later. **K. Casey**

9:35 CHED 225. Theories into practice in chemical and science teacher education. **J.W. Shane**

9:55 Intermission.

10:05 CHED 226. De-construction before construction. **G. Bhattacharyya**

10:25 CHED 227. Revisiting the problem-solving mindset: Reflections from the classroom. **D.E. Gardner**

10:45 CHED 228. Investigating the feasibility of integrating biopolymers as a STEM activity into an elementary education science methods course as a prompt to reveal understanding of polymer science concepts. **R. Ferguson**

11:05 CHED 229. Accessiblity of symbolic representations of chemical reactions. **A.L. Lewis**

11:25 CHED 230. Exasperating encounters in chemistry education scholarship while developing and implementing educational innovations for students enrolled in general chemistry. **T.J. Greenbowe**

Section B
New Orleans Marriott Convention Center
Blaine Kern A

ACS-CEI Award for Incorporating Sustainability into Chemical Education
Cosponsored by CEI and ENVR
S.O. Obare, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 231. 2011-2018: Advances in the personal and professional life of a materials scientist using sustainability as a platform for success. **A.E. Marteel Parrish**

9:05 CHED 232. Education for sustainable development in high school through inquiry-type socio-scientific issues. **R. Mamlok-Naaman**

9:35 CHED 233. Awareness and promotion of the roles of chemistry and chemical education in sustainability. **V.H. Grassian**

10:05 Intermission.

10:25 CHED 234. Relevant learning in science education: Research, development and implementation. **M. Hugerat**

10:55 CHED 235. Green & sustainable chemistry workshop for high school teachers. **J.E. Wissinger**, C. Knutson, C. Javner

11:25 Panel Discussion.

11:55 Concluding Remarks .

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Active Learning in the General Chemistry Curriculum

J.K. Robinson, *Organizer, Presiding*

8:30 CHED 236. Student attitudes and self-concepts in an active learning preparatory chemistry classroom utilizing the construction of explanations to promote understanding. **M.B. Atkinson**, S. Krishnan, L. McNeil, J.A. Luft, N.J. Pienta

8:50 CHED 237. Comparison of technology implementation used to integrate active learning into massive lecture courses. **A. Holton**

9:10 CHED 238. Active learning tools for general chemistry. **N. Tro**

9:30 CHED 239. Incorporating in-class active learning modules using online-accessed content in a collaborative learning classroom. **D.K. Wicht**

9:50 Intermission.

10:05 CHED 240. Combined instructional strategy and technology to engage and encourage students in active learning and teamwork discussion in integrated chemistry classroom activities. **N. Sanguantrakun**

10:25 CHED 241. Adding active learning to the first day of general chemistry lab. **E.P. Kippenhan**

10:45 CHED 242. Active learning *via* the "study buddy" system and team-presentations. **M. Ilies**

11:05 CHED 243. Chem101: Using smart suggestions as a novel digital input method for chemical nomenclature, formulae, and reactions to enable active learning assessments in first-year chemistry. **J.B. Weinberg**

11:25 CHED 244. Engaging general chemistry students with interdisciplinary investigations. **K.S. Owens**, A. Murkowski, H. Price, A. Johansen

Section D
New Orleans Marriott Convention Center
Blaine Kern E

State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry
Cosponsored by PRES
J.C. Warner, *Organizer*
I.J. Levy, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 245. Green chemistry theory & practice: Principle 1. From improving what is to inventing what could be. **J.C. Warner**, **P.T. Anastas**

9:35 Intermission.

9:45 CHED 246. Principle 2. From atom economy to circular economy. **S. Hunter**, R. Helling

10:05 CHED 247. Principle 3. Towards organic chemistry without organic solvents: The case for use of designer surfactants for safer organic reactions. **M. Cortes-Clerget**

10:25 CHED 248. Principle 4. Concepts of green chemistry and its role in the identification and design of safer chemicals and products. **P. Spencer**

10:45 Intermission.

10:55 CHED 249. Principle 5. Greener solvent alternatives for common medicinal chemistry applications. **J. Murray**

11:15 CHED 250. Principle 6. Delta S: An environmentally benign and worker safe asphalt additive. **J. Bianchini**

11:40 Concluding Remarks.

Section E
New Orleans Marriott Convention Center
Fulton

Research in Chemistry Education

J.H. Carmel, *Organizer*
M. Anzovino, *Organizer, Presiding*
J. Carmel, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 251. Peers promoting a growth mindset in the general chemistry laboratory. **H.B. Miller**, T. Knippenberg

8:55 CHED 252. Engaging students in green chemistry: Motivational outcomes of a green chemistry laboratory design in a first-semester general chemistry course. **L.J. Doody**

9:15 CHED 253. Developing assessment tasks for the scientific practices: Alignment, design, and testing. **J.H. Carmel**, E.M. Duffy, D.G. Herrington, M. Cooper

9:35 CHED 254. Implementation and evaluation of designated laboratory partnerships in an undergraduate chemistry laboratory. **D. Samarasekara**, D. Mlsna

9:55 Intermission.

10:10 CHED 255. Success in biochemistry: The GIG model and student backgrounds. **C.T. Cox**

10:30 CHED 256. Upper-division chemistry students' navigation and use of quantum chemical models: A fragmented conceptual landscape. **J. Beck**, M.N. Muniz

10:50 CHED 257. The utility of learning progressions in the undergraduate biochemistry curricular sequence. **A.M. Mercer**, A. Wolfson, S. Sutheimer, J.E. Lewis

11:10 CHED 258. The instructional profiles of undergraduate science classes: Characterizing teacher and student behaviors in over 2,000 classes. **J. Harshman**, M.N. Stains

11:30 Concluding Remarks.

Section F
New Orleans Marriott Convention Center
Blaine Kern B

Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

R.K. Boggess, *Organizer*
C.A. Burkhardt, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED 259. Assessing the impacts of the flipped classroom environment on student learning and motivation in chemistry. **J. Barbera**, M.M. Phillips

9:05 CHED 260. Improving STEM education through departmental action teams. **J.C. Corbo**, K. Falkenberg, C. Ngai, M. Pilgrim, G. Quan, D. Reinholz, S. Wise

9:30 CHED 261. Moving faculty from experimentation with to long-term adoption of engaged student learning in analytical chemistry. **R.S. Cole**, **T.J. Wenzel**, I. Brown

9:55 Intermission.

10:05 CHED 262. Promoting analogical reasoning in general chemistry laboratory experiments. **M.R. Bruce**, J.C. Walter, A.E. Bruce, A.C. Turner, D. Howard, S.R. Poll, C.D. Eaton

10:30 CHED 263. Technology-based support for students' representational competencies improves their learning of chemistry concepts. **M. Rau**

10:55 CHED 264. Visualizing chemistry with infrared thermography. **C. Xie**, A.T. Torelli

11:20 Intermission.

11:30 CHED 265. Building early career undergraduate research experiences at Pasadena City College. **V.I. Jaramillo**

11:55 CHED 266. NSF-Noyce at a primarily undergraduate institution: Initiating institutional change towards improving the pipeline of pre-service seconary STEM teachers. **D.L. Jacobs**

12:20 Concluding Remarks.

Section G
New Orleans Marriott Convention Center
Magnolia

Undergraduate Research Papers

Biochemistry

C.V. Gauthier, J.V. Ruppel, *Organizers*
N.L. Snyder, *Organizer, Presiding*

8:30 Introductory Remarks.

‡*Cooperative Cosponsorship*

8:35 CHED 267. Tapping in to the mystery of membrane protein expression. **C. Akley**, M.D. Rieth

8:45 CHED 268. Purification, crystallization, and characterization of essential *Mycobacterium tuberculosis* Rv3802. **C.M. Schreidah**, C.M. Goins, D.R. Ronning

8:55 CHED 269. Lysozyme denatuation in DMSO mixtures: A study on cryopreservation. **K. Rajesh**, K. Oh, C. Baiz

9:05 CHED 270. Decreasing PC on the surface of the LD correlates with altered protein binding and steatosis. **A. Jernberg**, A.K. Stoeckman, L. Listenberger

9:15 CHED 271. Remnant lipoprotein size distribution profiling via dynamic light scattering analysis. **A.V. Hernandez**, R. Chandra, B. Mellis

9:25 Intermission.

9:35 CHED 272. Visualizing gammaherpesvirus replication using viruses that encode fluorescently-tagged proteins. **D.N. Games**, S. Owens, J.C. Forrest

9:45 CHED 273. Elucidating the role of globin coupled sensors in *Pectobacterium carotovorum* virulence and quorum sensing pathways. **L. Briggs**, J. Burns, P. Jariwala, E.E. Weinert

9:55 CHED 274. Elucidating the roles of heme pocket residues in bacterial oxygen sensors. **P.G. Young**, S. Rivera, E.E. Weinert

10:05 CHED 275. Role of MRC2 in Wolff-Parkinson-White syndrome. **L. Acevedo-Soto**, X.H. Wehrens, S.K. Lahiri

10:15 CHED 276. Effect of an arginine to isoleucine active site mutation on *Escherichia coli* malate dehydrogenase enzymatic activity. **J. Zatorski**, B.J. Heyen

10:25 Intermission.

10:35 CHED 277. Synthetic biology: Production and utilization of aspirin producing bacteria. L. Gwyn, **M.J. Duckwall**

10:45 CHED 278. Photothermal effects of gold nanoparticles on A-375 skin melanoma cells. **A. Gorman**, T.J. Dominguez, M. Steiger, B. Mellis

10:55 CHED 279. Determination of the LD_{50} of muscle relaxants when combined with silver and gold nanoparticles on *Daphnia magna*. Y. Santos Vazquez, **P. Garcia Gonzalez**, **C. Cabrera Lopez**, E. Ferrer Torres

11:05 CHED 280. Human topoisomerase IIβ inhibition by new palladium (II) and platinum (II) complexes of a 2-acetylpyrazine tert-butylthiosemicarbazone ligand. **S.N. Grossarth**, S.G. Bowman, J.L. Hill, X. Jiang, E.C. Lisic

11:15 CHED 281. Inhibition of oxidative DNA-protein crosslinking via EGCG and quercetin. **P. Perez**, **J. Ordenana**, **M. Martinez**, E. Kroll

11:25 Concluding Remarks.

Section H
New Orleans Marriott Convention Center
Fleur De Lis

International Perspectives of Chemistry Education Teaching & Practice

A. Leontyev, *Organizer*
C.T. Cox, W.E. Schatzberg, *Organizers, Presiding*

8:30 CHED 282. International classrooms: An environmental perspective. **L. Abraham**

8:50 CHED 283. One country, two cultures: A multi-perspective view on Israeli chemistry teachers' beliefs about teaching and learning. **M. Hugerat**

9:10 CHED 284. Professional development and safety procedures in international chemistry education. **A. Farnsworth**, J.B. Nielson

9:30 Intermission.

9:45 CHED 285. Chemical education in India: Transformation through ages. **N. Bharti**, T.S. Kumbar

10:05 CHED 286. Global adaptation of a scientific writing course: From Missouri to China. **K. Yang**, **R. Glaser**, C. Guo

10:25 CHED 287. Upcoming international conferences in chemistry education in 2018. **W.E. Schatzberg**

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

Integrating Polymer Science in the Curriculum
Sponsored by POLY, Cosponsored by CHED and PMSE

Environmental Chemistry Undergraduate Education in the Classroom, Laboratory & Beyond
Sponsored by ENVR, Cosponsored by CHED

MONDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
Blaine Kern C

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry

M.H. Towns, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 288. Overview of the National Academies of Science, Engineering and Medicine (NASEM) report titled *Developing Indicators for Monitoring Undergraduate STEM Education*: Committee process and conclusions. **G.C. Weaver**

1:55 CHED 289. Inclusion in chemistry for students with visual impairments. **C.A. Supalo**

2:15 CHED 290. Fostering creativity and innovation: STEM to STEAM at South Dakota State University. **D.P. Cartrette**, D.M. Behl

2:35 CHED 291. Investigating the conversations of undergraduate research experiences. **S. Johnson**, G.M. Bodner

2:55 Intermission.

3:05 CHED 292. Modification of organic laboratory experiments to engage pharmacy students. **S. Holladay**

3:25 CHED 293. What's happening in laboratory? Encouraging meaningful learning in an electrochemistry laboratory. **A.J. Phelps**

3:45 CHED 294. Teaching assistants' perceptions and use of external representations when teaching acid-base titrations in introductory chemistry laboratory courses. N. Millick, **M. Orgill**

4:05 Intermission.
4:15 Introduction of Awardee.

4:20 CHED 295. Award Address (ACS Award for Achievement in Research for the Teaching and Learning of Chemistry Sponsored by the ACS Exams Institute). Changing how data are collected can change what we learn from discipline-based educational research. **G.M. Bodner**

Section B
New Orleans Marriott Convention Center
Blaine Kern A

US-Cuba Collaborations in Chemical Education

C.H. Atwood, R.M. Kelly, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 296. Developing relationships between Cuba and the American Chemical Society since 1998. **Z.M. Lerman**, M.Z. Hoffman

1:55 CHED 297. Progress report on DivCHED interactions with the Cuban Chemical Society. **C.H. Atwood**, R.M. Kelly

2:15 CHED 298. Some complementarities where Cuba and US can work together in science. **L. Montero**

2:35 Intermission.

2:45 CHED 299. Chemical education focused on biomedical research: The Cuban experience. **D. Garcia Rivera**

3:05 CHED 300. Ernest Eliel Workshop: US and Cuba collaboration in chemistry education and neglected disease drug discovery. **W.L. Scott**, A.A. Fuller, A.B. Dounay, J.G. Samaritoni, M.J. Odonnell, P. Dave, J. Sanchez, D. Tiano, D. Garcia Rivera

3:25 Intermission.

3:35 CHED 301. Environmental education from a chemical perspective. **M. Villanueva-Tagle**

3:55 CHED 302. Research to practice: Exploring ways to engage students with molecular animations. **R.M. Kelly**

4:15 CHED 303. Curricular and extracurricular activities that contribute to the research training of the chemistry graduate at the University of Havana, Cuba. **L.Y. Gonzalez**

4:35 Panel Discussion.
4:55 Concluding Remarks.

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Active Learning in the General Chemistry Curriculum

J.K. Robinson, *Organizer*
A. Murkowski, *Presiding*

1:30 CHED 304. Large lecture? No problem! Overcoming barriers to active learning to build excitement in large general chemistry courses. **J.K. Schwartz**, W.C. Pfalzgraff

1:50 CHED 305. Withdrawn

2:10 CHED 306. Strategies to promote active learning in a large general chemistry course. **J.K. Robinson**

2:30 CHED 307. Teaching mole concepts and stoichiometry using the active learning approach. **A.M. Bopegedera**

2:50 Intermission.

3:05 CHED 308. Overcoming obstacles to active learning in introductory chemistry for the health professions. **L.D. Frost**

3:25 CHED 309. Lessons learned in transforming my general chemistry course into full active learning under non-ideal circumstances. **M. Delgado**

3:45 CHED 310. Active learning when all your colleagues lecture: striking a balance. **S.M. Taylor**

4:05 CHED 311. Implementing a "What's In The Bottle Lab" guided inquiry lab in a first semester general chemistry class as an assessment tool for the general education program. **S.W. Carrigan**

4:25 CHED 312. Withdrawn

Section D
New Orleans Marriott Convention Center
Blaine Kern E

State-of-the-Art: Two Decades Advancing the 12 Principles of Green Chemistry
Cosponsored by PRES
J.C. Warner, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 313. Principle 7. Leveraging renewable feedstocks to drive consumer delight in fabric care products. **W. Shearouse**, **T. Cline**

1:55 CHED 314. Principle 8. NCDs–Powerful tools for reducing derivatives and realizing the green chemistry opportunity. **E. Stoler**

2:15 CHED 315. Principle 9. Catalysis: Catalytic coupling of phenol without using coupling reaction. **C. Li**, Z. Chen, H. Zeng, Z. Qiu, A.D. Huerta

2:35 Intermission.

2:45 CHED 316. Principle 10. Learning from nature how to make materials compatible with nature. **J.C. Warner**

3:05 CHED 317. Principle 11. An open discussion of unmet needs in analytical chemistry for green chemistry. **A.S. Cannon**, **I.J. Levy**

3:25 CHED 318. Principle 12. Can Green Chemistry prevent accidents or will chemistry always pose an inherent safety risk? **A.S. Cannon**

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3:45 Concluding Remarks.

Section E
New Orleans Marriott Convention Center
Fulton

General Papers

S.A. Fleming, *Organizer*
R.M. Kissling, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 319. Incorporating a peer-led approach for TA training. **C.T. Cox**

1:55 CHED 320. Reciprocal peer tutoring in general chemistry: Benefits to information retention and lowered student test anxiety. **D.W. Carpenetti**

2:15 CHED 321. Getting students to speak our language:Aadaptive tools for teaching nomenclature. J.P. Blinco, K. Mullen, **N.R. Boase**

2:35 CHED 322. Undergraduate teaching assistants as part of the teaching-service model in large introductory organic chemistry courses. **R.M. Kissling**

2:55 Intermission.

3:10 CHED 323. Withdrawn

3:30 CHED 324. Supplementary instruction and flipped classroom in organic chemistry. **S. Xie**

3:50 CHED 325. Implementation and analysis of a placement exam in first year chemistry courses at Henderson State University: Results, assessments, and outlook. **D. Bateman**, **B.A. Rowland**

4:10 Intermission.

4:30 CHED 326. Chemflix: A unique approach to combining traditional and online office hours for large lecture classes. **B. Turnpenny**, A.S. Silva, A.M. Haruk

4:50 CHED 327. Impact of an atoms-first approach on student outcomes in a two-semester general chemistry course. **C. Rezsnyak**

Section F
New Orleans Marriott Convention Center
Blaine Kern B

Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

C.A. Burkhardt, *Organizer*
R.K. Boggess, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 328. National Science Foundation programs that support undergraduate chemistry education. **T.D. Kim**, **D. Rickey**

2:00 CHED 329. The student participant perspective: Enhancing undergraduate research through international research experiences. **S. Hodges**, M.T. Fox, N. Brown, A. Niyongabo, J. Flores, R.A. Perez, J.A. Rosales, K.A. Jones, A. Keys

2:25 Intermission.

2:35 CHED 330. Development of Project ChemABLE (Active and Blended LEarning): Design, implementation, assessment, and dissemination of blended learning (flipped classroom) activities. **J.F. Eichler**

3:00 CHED 331. Alliance model for S-STEM project. **O. Jenda**, B. McCullough

3:25 CHED 332. Withdrawn

3:50 Intermission.

4:00 CHED 333. NSF-S-STEM: Iona DESIRE – Development of excellence in science through intervention, resilience, and enrichment. **S. Lee**

4:25 CHED 334. Development of an emporium styled general chemistry course. **M.A. Franks**, J. Emrani, M.M. Basti

4:50 Concluding Remarks.

Section G
New Orleans Marriott Convention Center
Magnolia

Undergraduate Research Papers

Inorganic, Bioinorganic & Materials Chemistry

J.V. Ruppel, N.L. Snyder, *Organizers*
C.V. Gauthier, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 335. Halogen to hydrogen bonding switch in complexes of iodo-, bromo-, and chloroform with anionic and neutral nucleophiles. **B. Watson**, O. Grounds, S.V. Rosokha

1:45 CHED 336. Synthesis and activation of small molecules by water-soluble iridium and rhodium complexes. **J.G. Knapp**, S.H. Schreiner

1:55 CHED 337. Application of air-stable palladium(II) precatalysts to Suzuki cross-coupling reactions and C-H activation of pyridine *N*-oxides. **J.R. Howard**, K.L. Barnett, K.H. Shaughnessy

2:05 CHED 338. Investigation and selection of inert substitutes for the energetic content of rolled steel cylinders in high energy laser effects research using differential scanning calorimetry. **J. Johnson**, D.E. Riegner

2:15 CHED 339. Predicting the properties of high oxidation state of some An(OH) x complexes. **A.C. Hartley**, Z. Lee, D.A. Dixon

2:25 Intermission.

2:35 CHED 340. Supercapacitor application of phosphorus and nitrogen co-doped carbon materials from renewable precursor materials. **S.P. Macchi**

2:45 CHED 341. Photoluminescence and stability enhancement of $CsPbBr_3$ NCs using amines and thiols for LED application. **A. Gunawan**, Z. Tan, Y. Wong, A. Ng

2:55 CHED 342. High-performance porphyrin-based dye-sensitized solar cells with iodine and cobalt redox shuttles. **J. Li**

3:05 CHED 343. Synthetic strategies for enhancing the properties of layered manganese dioxide for heterogeneous water oxidation catalysis. **L. Mohamad**, I.G. McKendry, M. Zdilla

3:15 CHED 344. Evaluating pellet-clad interactions using cerium oxide simulants and depleted thorium and uranium oxide thin films on zircaloy. **D. Perales**, T.J. Boyle, S. Briggs, K. Hattar, R. Dingerville

3:25 Intermission.

3:35 CHED 345. Synthesis of less toxic gold nanorods by using dodecylethyldimethylammonium bromide as an alternative growth-directing surfactant. **M. Blahove**, J. Xu, J.W. Stone

3:45 CHED 346. Cooperative catalytic metalloenzyme mimic with dinuclear metal ion binding sites. **G. Tegenkamp**, L. Carroll, A. Lajmi

3:55 CHED 347. Synthesis of a novel platinum(II) complex and investigation of its anticancer potential. **J. Jones**, D.J. Swartling, E.C. Lisic, G.A. Mullins

4:05 CHED 348. Degradation of tetracycline and tylosin using an iron modified titania photocatalyst. **J.L. Butler**, M. Clothier, J.E. Boyd

4:15 CHED 349. Development of a coumarin based molecular probe for trace metal ions. **R. Curtis**, K.J. Wallace

4:25 Concluding Remarks.

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Agricultural and Food Chemistry

Cosponsored by AGFD and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 350. An investigation into the characterization of unifloral honey samples by SNIF NMR. **C. Nicodemus**, A. Marchetti

CHED 351. Comparative analysis of date fruits from two different regions of the world. **S.F. Alharbi**, C. Chant

CHED 352. Identification of QTLs associated with consumer aesthetics and taste in *Vaccinium corymbosum*. **A. Hudson**, X. Li

CHED 353. Withdrawn

CHED 354. The role of nutritional components of vegetables in decreasing cancer incidence in Peru. **A. Edobor**, C. Quinonez, V. Viveros, B. Zavaleta, L. Nogaj, S. Deprele, L. Roberts

CHED 355. Determination of the effect of meringue under different conditions. **M.T. Nguyen**, E.D. Stemp

CHED 356. Quantitative analysis of arsenic in basil. **B. Corporon**, R. Nava, K. Pollok, A.M. Bray

CHED 357. Fabrication of polyvinyl alcohol thin film synthesized with gold nanoparticle and β-cyclodextrin for detection of parathion. **M. Koh**, A. Deckert

CHED 358. Determination of allelopathic compounds in sugarcane field residue extracts. **K.J. Kraemer**, J. Zhu, D.S. Landrum, C.L. Webber, P.M. White, D. Wayment

CHED 359. Effect of the decaffeination process on chlorogenic acid levels in coffee beans using UV/VIS spectroscopy. **D. Patel**, S.W. Carrigan

CHED 360. Analysis of sugarcane billet seed treatment chemicals in agricultural soil by HPLC. **K.A. Torres**, H.J. Ledet, C.L. Webber, P.M. White, **D. Wayment**

CHED 361. What the taffy: Tensile strength relative to corn syrup viscosity. **U. Wilkerson-Dixon**, P.A. Brletic

CHED 362. Color me caramel: Impact of milk source on taste and physical behavior. **E. Chambers**, P.A. Brletic

CHED 363. Study of the anitmicrobial activity of honey against antibiotic resistant bacteria. **L. Andrews**, N.S. Green

CHED 364. Isolation and structural ellucidation of color from the mushroom *Polyozellus multiplex*. **O.Z. Schaefer**, A. Kleinschmit

CHED 365. Immobilizing acetolactate decarboxylase to eliminate diacetyl from beer. **J. Hitt**, R.A. Hunter

CHED 366. Antibacterial activity of pyrogallol-based polyphenols and compounds in wine. **K.A. Thomas**, M.A. Fisher

CHED 367. Rates and levels of saturated, monounsaturated, and polyunsaturated dietary triglyceride oxidation. **A. Verlander**, E. Csuhai

CHED 368. Examining and preventing zein protein aggregates. **L. Sanchez**, L.J. Moore

CHED 369. Qualitative analyses of local craft spirits compared to common large brands using gas chromatography-mass spectrometry. **C. Shinn**, A. Pilchowski, J.A. Trischman

CHED 370. Comparison of growth and energy content of *Spriodela polyrhiza* and *Lemna minor*, two potential biofuel sources. **R.M. Robinson**, **P.S. Whitehead**, P.W. Sharp, S. McKim, N.L. Paiva

CHED 371. Determination of the quality of phytopharmaceuticals and dietary supplements of products that are marketed in Costa Rica. **J. Ramirez Torres**, R. Murillo Masis, J. Quesada Espinoza

CHED 372. Extraction and determination of phytochemical and antioxidant activities of watermelon seed oil (*Citrullus Lanatus*). **S.A. Aderibigbe**, G.K. Oloyede

CHED 373. Flavor chemistry of Texas bourbon: Detection and separation of flavonoids by dispersive liquid-liquid micro-extraction (DLLME). **B. Pelletier**, **T. Craig**, K. Drake

CHED 374. Chemistry of baking: Analyzing volatile compounds in basic bread. **E.R. Currens**, L.J. Moore

CHED 375. Enhanced antioxidant activity in hypertriglyceridemic serum measured through a ferric reduction assay. **A. Rasool**, R. Chandra, S. Ghaoui

CHED 376. Variation of chemical composition of coffee in relation to time after roast. **C. Morder**, E.A. Baldauff

CHED 377. Measuring calcium uptake and release by *Saccharomyces cerevisiae* throughout the fermentation process. **N. Mesloh**, L. Benedict, M. Ackerman

CHED 378. Analysis of chemical and physical properties of west Tennessee

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honeys. **B. Barrett**, A.H. Shelton

CHED 379. Quantitation of dimethyl sulfide in beer using headspace flame-photometric detection and gas chromatography/mass spectroscopy. **N. Bice**, L. Benedict, Z. Bodah

CHED 380. Isolation and structure elucidation of alteichin, a fungal natural product that inhibits *Xylella fastidiosa*, the bacterium that causes Pierce's Disease. **S. Davis**, **S. Thompson**, **V. Berry**, **C. Brandenburg**, P. Rolshausen, C. Roper, K.N. Maloney

CHED 381. Xanthohumol derived from hops *Humulus lupulus*: Application in oral health. **A.R. Chavez**, W. Deutschman

CHED 382. Application of the atomic absorption spectrophotometer to determine the bioavailability of cadmium in *Raphanus*. **J. Stanley**, K.E. Garrison

CHED 383. Analysis of catechin and methylxanthine composition in tea (*Camellia sinensis*) by high pressure liquid chromatography. **C. Hull**, S. Hughes, R. Jalbert, P. Sheumaker, D. Choffnes

CHED 384. Fate of calcium, magnesium, and zinc throughout the brewing process. **P. Keehn**, L. Benedict, Z. Bodah

CHED 385. Induced monoterpene defense strategies in eastern white pine against blue-stain fungi *Ophiostoma minus*. **M.T. Phan**, **R. Funai**, **A. Arango-Velez**, **S. Chakraborty**

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Analytical Chemistry

Cosponsored by ANYL and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 386. An optimized method for the identification of pesticides in cannabis products using GC/MS with AMDIS. **K. Cochran**, H. Harris

CHED 387. Carbon based anode for microbial water treatment system. **A. Gonzalez**, M. Morales, C.R. Cabrera

CHED 388. Electrochemical characterization of HSA-heme-imidazole complexes towards future nitrite reductase activity. **A. Kelly**, J.A. Bennett, M.I. Galinato

CHED 389. Viability of $Ni(OH)_2$ and CeO_2 as electrocatalysts for oxygen evolution in metal-air batteries. **R. Lopez**, D. Mitra, S. Narayan

CHED 390. Developing thermal devices for donor-acceptor columnar liquid crystals alignment and analysis. **G. Pleitez Gomez**, J. Reczek

CHED 391. Quantifications of epicatechin content in brewed cocoa and factors that influence extract efficiency. L.B. Thompson, **S. Chen**

CHED 392. Determination of lead and other heavy metal contamination of maple syrup produced in St. Lawrence and Chittenden counties. **P. Park**, M.C. Skeels

CHED 393. Identification of volatile organic compounds present in decaying chicken organs using SPME-GC/MS. **A. Flotteron**, **T.N. Lewis**, M. Sabo

CHED 394. Investigating the impact of lipid formulations on the aggregation and behavior of amphotericin B. **T.N. Lewis**, K. Higgins, G. Sarabia, T.R. Calhoun

CHED 395. Development and validation of a method using QuEChERS and liquid chromatography-mass spectrometry for atrazine determination. D.J. Dayfield, C.R. Fiorido, **K.S. Lambert**, K.M. Marji, K.M. Marshall, D.N. Maxwell, I. Sayed, V.C. Torres, K.E. Yacoo, R.M. Belanger, E. Roberts-Kirchhoff, K.R. Evans

CHED 396. Colorimetric array for pH determination of soil samples. **R. Wiederkehr**, T. Bilinski, R.M. Burks

CHED 397. RGB image analysis for colorimetric real-time reaction monitoring. **C. Azaldegui**, L. Gaunt, R.M. Burks

CHED 398. Development of a nitrate/nitrite determination in salt water using an azo dye method to study the effects of titanium dioxide nanoparticles in the nitrogen cycle of *Favites Pentagona* Coral environment. M.O. Montes, **M. Wood**

CHED 399. Surface-enhance fluorescence enhancement studies on electrochemically deposited silver fractal-like structures. **D. Rios**, J. Yarbrough, R. Fudala, I. Gryczynski, T. Shtoyko

CHED 400. Increasing ICP-MS sensitivity. **R. Peterson**, W.E. Schatzberg

CHED 401. Control over the alignment of naphthalene diimides on a Langmuir-Blodgett trough. **X. Gao**, A. Edwards, J.J. Reczek

CHED 402. Capillary electrophoresis of glycosaminoglycans with indirect detection using naphthalene sulfonates. **L.R. Kuhn**, J. Fasciano, R.T. Taylor, N.D. Danielson, S. Shamsi

CHED 403. Effect of pH and counterion on chiral recognition of undecylenic leucine surfactant. F.H. Billiot, E. Billiot, K.F. Morris, Y. Fang, **A. Risley**

CHED 404. Physical properties of undecyl valine surfactant at different pHs. **S. Subniak**, F.H. Billiot, E. Billiot, K.F. Morris

CHED 405. Study of amino acid surfactant undecyl leucine using diffusion ordered spectroscopy technique. **M. Aleksich**, K.F. Morris, E. Billiot, F.H. Billiot

CHED 406. Construction and testing of a 2D photocurrent scanning station for the evaluation of thin film ternary metal oxide water-splitting photocatalysts. **A. Battiste**, S.M. Drew, K.L. Mertz

CHED 407. Detection of nitrotoluenes in canine fur samples using GCMS/PSI-probe. **H. Maruskin**, G. Patterson

CHED 408. Blood alcohol and arson investigation using SPME fibers. **C. Parker**, R. Montgomery

CHED 409. Construction and testing of an inexpensive spin coater. **K.L. Mertz**, S.M. Drew, A. Battiste

CHED 410. Use of principal component analysis and hierarchical clustering analysis to evaluate fingerprint residues. **R.B. Thomas**, T.J. Kuhns, S. Zentz, D.S. Egolf

CHED 411. Photocatalytic degradation of fenofibrate and other pharmaceuticals. **S.K. Bard**, L.A. Tom

CHED 412. Biodiesel synthesis and analysis: Qualitative comparison. **E. Millward**, **J. Didelot**, M.B. Jacobs, S. Ahsan

CHED 413. Electrochemical investigation of facilitated terbium(III) transfer at micro-liquid/liquid interfaces. **Z.T. Vander Tuin**, S.N. Thorgaard

CHED 414. Identification and quantitation of synthetic cannabinoids by gas chromatography-mass spectrometry. **D.M. Biller**, T. Frielle

CHED 415. Detection of miRNA 92a as a viable means of elucidating disease states. **K. Thomas**, A. Gee, N. Nguyen, M.F. Ali

CHED 416. Determining the age of a bloodstain through ultraviolet visible spectroscopy. **T. Yurasits**, G.P. Foy, K. Opel

CHED 417. Screening method development for the identification of nontargeted designer drugs by GC-MS^n and LC-MS/MS. **M.S. Fulmer**, J.O. Boles, T.H. Boles

CHED 418. Temperature-dependent rotational correlation times for liquid phase acetic acid. **C. Straub**, J.A. Goodnough

CHED 419. Analysis of sulfate levels in drinking water, wastewater, and natural water using UV-vis spectroscopy. **L.A. Cutler**, G.P. Foy

CHED 420. Investigation of heavy metal content in sand following beach renourishment in South Carolina. **L. Howe**, J.M. Fautch

CHED 421. Method validation of titanium dioxide nanoparticle analysis. **C. Kristoff**, M. Ellington, L.A. Holland

CHED 422. Effects of fingerprint degradation on the success of development methods. **G. Vitale**, K. Opel

CHED 423. Surface-enhanced Raman spectroscopy (SERS) analysis of western African artifacts. **M.C. Marshall**, J.M. Esson

CHED 424. Evaluation of conductive filaments through 3D printing technology and electrochemical experimentation. **M.J. Sheaff**, H.D. Whitehead, G. LeBlanc

CHED 425. Analysis of different types of inks by UV-vis spectrometry. **R.C. Pendley**, R. Fietkau

CHED 426. Elemental profiling of gunshot residue using total-reflection X-ray fluorescence spectroscopy. **M.E. Oliva**, N. Homburger, L. Huang, J. Berger

CHED 427. Analysis of metal content in ore from Alabama's first iron mine. **C. Boyd**, **S.A. Burton**, M.J. Kendrick-Murphy

CHED 428. Improving the fabrication of carbon fiber microelectrode sensors. **D.R. Miller Jr.**, R.B. Keithley

CHED 429. Simple analytical techniques for small breweries. **M. Symcox**, J. Sabo, G. LeBlanc

CHED 430. Multiplexed point-of-care breast cancer marker detection system in human body fluids. **B.S. Dang**, P. Pham, Z. Huang, Z. Wang

CHED 431. Determination of the metal content in deer hooves and duck feet: Sentinels of health, nutrition and the environment. **J.C. Reynolds**, L. Gildea, L. Selph, M.J. Kendrick-Murphy

CHED 432. Testing IR spectroscopy as an alternative method for water content determination in aviation fluids. **M.E. Cook**, G.T. Eldridge, R.K. Larsen

CHED 433. Glucose biosensing integrating aerogel components. **C.J. Brady**, **D. Saad**, N. Kosciuszek, M.C. Leopold, A.S. Harper-Leatherman

CHED 434. Uptake of nitrate and phosphate ions by native, non-invasive plant species. **M.B. Strickley**, **W.R. Cummins**, R.L. Bretz

CHED 435. Determination of pK_a's of various glycine metal complexes by NMR. **T. Tran**, T.K. Ellis, J.C. Henrikson

CHED 436. Thermal behavior of carbamazepine polymorphs characterized by variable temperature NMR. **S. Stuchell**, J.T. Hosfelt, R. Iuliucci

CHED 437. Characterization and application of field deployable thermodenuder for atmospheric aerosol volatility measurements. **G. Burke**, K. Kolesar, K.A. Pratt, M. Gunsch

CHED 438. Analysis of sitagliptin in milk using gas chromatography mass spectrometry. H.N. Currie, **B. Day**

CHED 439. Preparative chromatography of polyphenolics using size-exclusion and reverse-phase chromatography. **B. Trimmer**, P.V. Maciejczyk, G. Bradley

CHED 440. Determining the nutrient health of the Oconee River. **D. Cook**, C.H. Lisse

CHED 441. Determination of pesticide residues in soil. **N. Bauer**, C.H. Lisse

CHED 442. Quantitation of metal ions in surface waters in Southeastern Wisconsin. **L. Hall**, C.A. Blaine

CHED 443. Towards the development of a bioadhesion-resistant self-assembled scaffold for the chemical attachment of enzymes to gold surfaces. **J. Duchesneau**, B.W. Gregory

CHED 444. Development of metal ion specific sol-gel targets for trace metal total reflection X-ray fluorescence analysis. **L. Skolrood**, A.M. Butler, A. Arndt, R.N. Dansby-Sparks

CHED 445. Ion formation from inorganic salt aerosols in single-particle mass spectrometry. **A.E. Watson**, N. May, M. Gunsch, N. Olson, A.P. Ault, K.A. Pratt

CHED 446. Electrochemical determining of acetaminophen with multi hydrogen bonding manipulated single-molecule recognition. **P. Pham**, Z. Huang, K.E. Riley, Z. Wang

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CHED 447. Synthesis and characterization of fragrance encapsulated in silica sol-gels. **J. Fortwengler**, C.H. Lisse

CHED 448. Examining atrazine accumulation and histological changes in the hepatopancreas of crayfish post-exposure. **D.J. Dayfield**, **D.N. Maxwell**, **V.C. Torres**, **K.E. Yacoo**, K.S. Lambert, I. Sayed, C.R. Fiorido, K.M. Marji, K.M. Marshall, K.M. Barawi, N.K. Abraham, R.M. Belanger, E. Roberts-Kirchhoff, K.R. Evans

CHED 449. Validation of grazing angle ATR-FTIR for analysis of self-assembled monolayers. **R. Araj**, A. Radadia

CHED 450. Optimizing an SPE-GC-MS/MS method for wastewater-based epidemiology. **G. Kroening**, **J. Aquino**, K.J. Bisceglia

CHED 451. Liquid-liquid extraction and analysis of the antioxidant, resveratrol, from various red and white wines. **C.L. McGlocklin**, F.C. Mayville

CHED 452. Development of a cost effective alternative for spatter blood. **S. Choi**, K. Opel

CHED 453. Cation exchange-solid phase extraction protocol for the isolation and analysis of alkaloids in poison frogs. **K.S. Gleason**, **J.R. Sanders**, **N.R. Andreasen**, **J.M. Smith**, K.T. Bell, R.W. Fitch

CHED 454. Determining the effects of *in vitro* adulterants to valium drug tests. **R. Revuelta**, K. Opel

CHED 455. Spectrophotometric investigation of the suitability of indole for the determination of nitrite. D.A. Habboush, **M. Aboueissa**

CHED 456. Assessment of trace element content in fingernails: Association with physical activity in female college students. **M. Clausell**, **H.M. Parks**, M.J. Kendrick-Murphy

CHED 457. GC analysis of carburetor component reactions with gasoline. **E. Wesolowski**, T.R. Burkholder

CHED 458. Fluorescence quantitation of human lipoproteins through anion exchange HPLC. **R.H. Montoya**, **N. Nguyen**, R. Chandra

CHED 459. Separation of steroid isomers by ion-mobility mass spectrometry for forensic and metabolomics applications. **T. Martin**, A.L. Rister, E.D. Dodds

CHED 460. Isolation of potential antifungal compounds in *Aloe cameronii*. **A.N. Colah**, **L.N. Raess**, M.R. Lee, R.L. Bretz

CHED 461. Scratching the surface: Applications of AFM-IR in indoor surface chemistry. **S.P. Schwab**, V.W. Or, V.H. Grassian

CHED 462. Determination of pesticide residues in vegetable samples. **E. Bullington**, C.H. Lisse

CHED 463. Molecular fingerprinting of K562 human leukemia cells via MALDI-TOF mass spectrometry. **T. Lyons**, E. Hong, A. Gaito, L. Cintron-Rivera, L. Dupree, C.J. Andersen, A.R. Van Dyke

CHED 464. Lead in avian eggshells and egg contents. **M. Freeman**, R.C. Dudek

CHED 465. Qualitative and quantitative analysis of heavy metals in cigarettes via inductively coupled plasma optical emission spectrometry. **D.T. Bortz**, F.C. Mayville

CHED 466. Determination of bisphenol A (BPA) in infant oral hygiene devices using fluorescence spectrophotometry. **K.A. Thomason**, S.E. Hubbard

CHED 467. Colorimetric analysis of nicotine in cigarettes via ultraviolet-visible spectrometry. **D.T. Bortz**, F.C. Mayville

CHED 468. Relating the chemical and morphological characterization of plaster cast statues to durability. **J.N. Ferreri**, A.S. Harper-Leatherman, K. Schwab, J. McGovern, M.A. Kubasik

CHED 469. Characterization of a paper-based analytical device for low molecular weight and unfractionated heparin. **C.E. Norris**, J.M. Esson

CHED 470. Further studies of the analytical method for the determination of phenylarsonic acid. **R. Herbers**, B.M. Hopkins

CHED 471. Mass spectral identification of isopropyl acetate in Louisiana flood water. **J. Shelby**, D. Oldendorf, D.P. Gautreaux

CHED 472. Development of a methodology for the characterization of primitive meteorites by infrared spectroscopy. **J. Coovert**, S.F. Wolf

CHED 473. Measurement of urinary sulfate levels in pigs by conductometric titration. **S.N. Crews**, **J. Garcia**, L.D. Schultz

CHED 474. Detection and determination of food residues in Native American pottery. **K. Plotzke**, J. Sebree, D. Gaff

CHED 475. Isolation of aptamers for detection of *Renibacterium salmoninarum* in water. **M.D. Hoppe**, B.G. Staebler-Siewell, B. Peterson, A.G. Cavinato

CHED 476. Effects of soil chemistry on the distribution and abundance of sundews (*Drosera* sp) on the Craven Community College campus. **C.A. Hardtle**, D.W. Carpenetti, Q.E. Lupton

CHED 477. Synthesis and analysis of impure functional group substituents of dihydrodeoxymorphine "krokodil". **D. Verret**, D. Oldendorf, D.P. Gautreaux

CHED 478. UPLC/ESI-TOFMS method development for cocoa origin classification. **L.W. Monroe**, R.E. Sours, S.E. Stitzel

CHED 479. Effects of blood degradation in presumptive testing for blood evidence. **E. Nikolaus**, K. Opel

CHED 480. One year later: GC-MS study of water quality following a 1000-year flood in the Baton Rouge region. **A. Vick**, D. Oldendorf, D.P. Gautreaux

CHED 481. Optimization of disulfide bond reduction for use in point-of-care microfluidic-based devices with applications in early cancer diagnosis. **S. Cook**, C.T. Culbertson

CHED 482. Analysis of the chemical composition of spinach after exposure to glyphosate. **S. Glynn**, D. Oldendorf, D.P. Gautreaux

CHED 483. Amphibian chemical ecology: Method development in natural product identification. **E. Doe**, **A. Poltronetti**, T.P. Umile, L. Rollins-Smith, K.P. Minbiole

CHED 484. Identification of ethyl isobutyl ether in Louisiana flood water using GC/MS. **S. Deynzer**, D. Oldendorf, D.P. Gautreaux

CHED 485. Identifying the manufacturer of unknown fingernail polishes. **C. Carbajal**, G. Naisbit

CHED 486. Identification of volatile organic compounds in flood waters using GC/MS. **P. Prevost**, D. Oldendorf, D.P. Gautreaux

CHED 487. Electrochemical comparison of dicyanoferriprotoporphyrin-modified carbon and Pt microelectrodes for selective H_2S detection. **H. Pharathikoune**, J.A. Bennett

CHED 488. Aerosol deposition of metal-organic framework thin films. **B. Barrett**, J.E. Shankwitz, A. Hauser, G. Szulczewski

CHED 489. Development of a raspberry Pi and Arduino-based thermal controller and desorber for GC/MS vapor analysis. **D. Holden**, G. Patterson

CHED 490. Precipitation SELEX: Selection and study of DNA aptamers that template calcium phosphate mineralization. **K. Meserve**, A.E. Gerdon

CHED 491. Qualitative determination of the adherence of VOCs to building materials. **J. Turner**, C.H. Lisse

CHED 492. Thermodynamic studies of gas-phase equilibrium in MALDI-MS. **M.H. McMinn**, L.A. Elliott, G.R. Kinsel

CHED 493. Kinetic analysis of thermal degradation in high temperature high-performance liquid chromatography: Acetylsalicylic acid. **B. Levine**, J. Arena

CHED 494. Evaluation of aroma compounds of small-batched, unaged wheated whiskey. **A.V. Horton**, N.E. Huddleston

CHED 495. Determination of quench in Cherenkov counting of soil samples. **R. Myers**, W.B. Connick, S. Herman, S. Glover, H. Spitz

CHED 496. Investigating the Beer-Lambert law in a cavity-enhanced spectroscopic method. **Z.R. Thornburg**, K.J. Feierabend, S. Lehman

CHED 497. Analysis and verification of alternate industrial volatility testing methods. **B. Pinkley**, S. Dubecky, R. Johnston

CHED 498. Energy dispersive X-ray fluorescence analysis of a series of copper-based coins of the Indo-Parthian king Gondophares I. J. Pothoof, **M. Bhagwagar**, **T. Ngo**, M.A. Benvenuto

CHED 499. Quantum dot probes for protein biomarker detection. **K.A. Medley**, A.P. Cordner, K.L. Parks, M. Yu

CHED 500. Voltammetric detection of lead and cadmium using a cloud point extraction. **A. Keating-Zaid**, **T. Martin**, **M. York**, A.F. Bange

CHED 501. Immobilization of porphyrins in sol-gel matrices. **M. Schellman**, C.H. Lisse

CHED 502. Development of simple quantum dots-based bioassays for protein biomarker detection. **K.L. Parks**, A.P. Cordner, K.A. Medley, M. Yu

CHED 503. Fluorescence intensity alteration of quantum dots by protein biomarkers. **T. Parks**, A. Rowley, M. Yu

CHED 504. Chemical analysis of artistic and cultural heritage objects from western Africa. **M.H. Tran**, J.M. Esson

CHED 505. Analysis of vibrational modes of chemically modified tone wood. **M.M. Flesch**, J.D. Rollison, C. Hanson

CHED 506. Evaluating the water quality of selected polluted sites in New York City. **J. Zapata**, E.E. Mojica, L. Birney

CHED 507. Binding capacity of nanoceramics with sulfa drugs. **G. Iannone**, E.E. Mojica

CHED 508. Phenol content and antioxidant activities of several commercial tea samples. **A. Villaggi**, E.E. Mojica

CHED 509. Binding interaction of nanoceramics (metal oxides) with human serum. **T. Nolan**, E.E. Mojica

CHED 510. Sample preparation and analysis of PAHs (polycyclic aromatic hydrocarbons) in milk samples. **L. Wyan**, E.E. Mojica

CHED 511. Forensic soil analysis by subtractive FTIR spectroscopy. **C.A. Haines**, S. Davis

CHED 512. Stability of AH-7921 and U-47700 in polar organic solvents. **M. Murphy**, K. Scott

CHED 513. Persistance of gasoline deposited on typical footwear. **A. Narehood**, M. Cipoletti

CHED 514. Determining levels of bisphenol A leached into water from thermal receipt paper using fluorescence spectrophotometry. **M. Bolin**, S.E. Hubbard

CHED 515. Determination of erythromycin in fish tissue by liquid chromatography with UV detection. **C.D. Cunningham**, **C.A. Freeman**, E. Lavadour, G. Rodriguez, A.G. Cavinato

CHED 516. Two-dimensional vibrational analysis of tone wood in string instruments. **J.D. Rollison**, M.M. Flesch, J. Sebree, C. Hanson

CHED 517. Development of analytical methods for butylorganotin compounds. **G. Dangel**, A. Hardee, B.M. Hopkins

CHED 518. Measurement of sulfate levels in west Texas groundwater by conductometric titration, ion chromatography, and SulfaVer methods. R. Srinivasan, **W.M. Grumbles**, **J. Garcia**, L.D. Schultz

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CHED 519. Characterization of DNA aptamers for sensor development. **H.M. Breen**, **J.K. Carter**, A.G. Cavinato

CHED 520. Chromatographic analysis of amphetamines in biological samples. **L. Reilly**, E.E. Mojica

CHED 521. Characterization of bee propolis from Bulgaria and Serbia. **J. Farshi**, E.E. Mojica

CHED 522. Optimization of surface chemistry of thiol-ene crosslinked organo-silica monolithic columns and their application in capillary liquid chromatography. **A. Burkus-Matesevac**, Z. Zajickova, F. Svec

Section H
ErnestN. Morial Convention Center
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Undergraduate Research Posters

Biochemistry

Cosponsored by BIOL and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 523. Compensatory mutations in the M13mp phage series. **R. Aldakhlallah**, **L. Gray**, **M. Salemi**, **A. Sylvia**, M. Hall

CHED 524. Cinnamic aldehyde conjugate-based nanoparticles for the treatment of arterial restenosis. **C. Pérez Verdejo**, E. Valentín Méndez, H. Lutz, N.E. Buglak, W. He, E.M. Bahnson

CHED 525. Construction of a more virulent lacZβ-containing M13 phage vector. **E. Botelho**, **G. Mahame**, M.F. Hall

CHED 526. Molecular mechanics investigation of the potential binding sites of cannabinoid derivatives on the human CB1 and CB2 receptors. **W. Smith**, M. Dorko

CHED 527. Effect of citral on apoptosis in human melanoma cells. K.S. George Parsons, **M.K. Johnson**

CHED 528. Characterization of somatic mutations found in polymerase kappa. **C.E. Fitzgerald**, J. Andrade, S. Lone

CHED 529. Role of signaling lipid phosphoinositides PI(3,4,5)P_3 and PI(3,4) P_2 In neural growth cone invadosomes. **A. Bali**, C. Short, T. Gomez

CHED 530. Characterization of the phosphoribsyl transferase ToyH; An essential enzyme in the production of the antibiotic sangivamyin. **C.J. Aston**, N.A. Bruender

CHED 531. Peptide-based targeting of antimicrobial conjugates to sporulated *Bacillus anthracis.* **B. Cooper**, S. Campbell, R. Giorno-McConnell, S. Poh

CHED 532. Progress In synthesizing a novel bromo-substituted aurone as a cyclooxygenase-2 inhibitor. **S. Forbes-Pentecost**, S. Stephenson, C.J. Mills

CHED 533. Identifying KDAC5 substrates. **J. Carmon**, T. Toro, T. Watt

CHED 534. Investigating the DNA protective effect of Mn^{2+} import in *E.coli* strain DH5-alpha and CSH 104. **A. Edobor**, B. Cadena, D. Duran, **P.E. Lee**

CHED 535. Characterization of the inducamide biosynthetic pathway. **J. Korchak**, A. Lane

CHED 536. Biosynthesis of diketopiperazine natural products from unnatural amino acids. **R. Lopez**, C. Webb, R. Viswanathan, A. Lane

CHED 537. Synthesis, characterization and biological testing of methylated flavonoid derivatives as potential cyclooxygenase-2 inhibitors. **L. Co**, C.J. Mills

CHED 538. Extraction, characterization and screening of plant extracts used in the traditional medicine of Zambia. **S. Stephenson**, A. Cowart, S. Mutiti, M. Mutiti, C.J. Mills, S. Mutiti

CHED 539. Calcium, caspase, and cancer: Connections through circular dichroism spectroscopy. **S. Hethcox**, L. Love, A.L. Stewart, M. Davis Mcgibony

CHED 540. Investigations of protein conformational changes as a signal for apoptosis. **L. Love**, S. Hethcox, A.L. Stewart, M. Davis Mcgibony

CHED 541. Synthesis and characterization of novel flavonoid derivatives as tau self-aggregation inhibitors for the treatment of Alzheimer's disease. **S. Martin**, **G.A. Layfield**, C.J. Mills

CHED 542. Using high-performance liquid chromatography in determining a drug's ability to permeate the blood-brain-barrier for the treatment of Alzheimer's disease. **P. Espinosa**, C.J. Mills

CHED 543. Development of screening strategy for potential antibiotics. **B. Grosso**, S.M. Kennedy, A.L. Miller

CHED 544. Exploring substrates for lysine deacetylase 7. **K. Nichols**, T. Toro, T. Watt

CHED 545. Role of N346 in class C beta-lactamases. **L. Hinojos Madrid**, S.T. Lefurgy

CHED 546. Role of Trm732 in tRNA modification and cell growth. **J.K. Ziebro**, D. DiVita, H.E. Sizemore, M. Guy

CHED 547. Microgravity-mediated resistance of *Helicobacter pylori* to stress. **L. Grafton**, J. Truong, D. McGee

CHED 548. Evolution of cephamycinase activity in Class C beta-lactamases. **H.W. Servius**, S.T. Lefurgy

CHED 549. Synthesis of metal chelating nucleosides. **J. Bernal**, N.J. Greco

CHED 550. $Os(phen)_2dppz^{3+}$: An osmium metallointercalator that selectively oxidizes guanine oxidation products. **E. Kroll**, **J. Dominguez**, E.D. Stemp, K.R. Miller, Z.A. Esguerra, M. Safaeipour, M. Bekarian

CHED 551. Role of the deep brine layer in mercury cycling within the Great Salt Lake. **A. Piskadlo**, F. Black, S. Yang, R. Rowland, W.P. Johnson, A. Reynolds, A. Robert, G. Pandey, C. Rumsey

CHED 552. Inhibition of DNA oxidative damage by green tea in vitro and in human melanoma cells. **E. Kroll**, **M. Serrano**, E.D. Stemp, M. Martinez, J. Ordenana, P. Perez, L. Nogaj

CHED 553. Solubility studies and investigation of delivery of a curcumin-β-cyclodextrin inclusion complex using a microdialysis probe. **E. Loch**, H.J. Fletcher

CHED 554. Modification of hOSBP ligand binding domain. **E. Wilson**, A. Burgett, N. Kothapalli

CHED 555. Analysis of DNA damage in *Bacillus subtilis* induced by nanoscale complex metal oxide. **K. Hoang**, **T. Pho**, T.A. Qiu, A. Carra', M.N. Hang, R.J. Hamers, S. Balbo, C.L. Haynes, V. Feng

CHED 556. KDAC4 specificity and mechanism. **D. Hill**, T. Toro, T. Watt

CHED 557. Synthetic chalcones as inducers of the Nrf2/Keap1 transcription factor-mediated signaling pathway. **J. Haseleu**, M. Hillwig

CHED 558. Effects of liopfectamine MessengerMAX on hybridization state of DNA-based molecular beacons. **F. Sanchez-Conde**, C.H. Battle

CHED 559. Role of Notch 2 receptor signaling during eosinophil activation in a house dust mite model of inflammatory asthma. **C.L. Olbrich**, E.D. Howard, E.W. Cornwell, L.A. Spencer

CHED 560. Using FRET to elucidate the lipid trafficking mechanism of SP-B C and N terminal peptides in comparison with KL_4. **K. Kroning**, O. Braide-Moncoeur

CHED 561. Biochemical characterization of YbeY from *E. coli.* **A. Krysztofowicz**, B. Smith, G. Culver

CHED 562. Elucidation of amino acids regulating the species-selective activation of TRPM8 by coal fly ash particles. **H. Peterson**, C. Reilly, J.G. Lamb

CHED 563. Synthesis and antibacterial testing of terpene-substituted Cefotaxime. **B. Hunt**, **A. Maroney**, S.A. Brouet

CHED 564. Effects of expression of myoglobin in *E. coli* on the bioavailability of iron. **C. Carroll**, T. Sivy

CHED 565. Reduction of high-valent iron species in hemoglobin: Implications for heart disease. **J. Ejim**, H.R. Williamson

CHED 566. Determining the effect of surfaces on islet amyloid polypeptide and prion peptide aggregation. **C.M. Yip**, A.M. Schenck, E.A. Yates

CHED 567. Differential expression of glycine receptors in the globus pallidus, thalamus, and striatum. **J.A. Paul**, M. Miranda

CHED 568. Protein kinase inhibitor H-89 blocks a metabolic switch in cells lacking the tumor suppressor p27kip1. **R. Khattab**, A. Alarabi, R. Sheaff

CHED 569. Glucose control of a metabolic switch in cells lacking the tumor suppressor p27kip1. **S. Sullivan**, R. Sheaff

CHED 570. Pharmacokinetic studies of aspirin degradation in the presence of enzymes. **A. Wagoner**, R.V. Macri

CHED 571. FRET-detected catalysis as a method to study RNA folding. **J. Pfeilstifter**, A. Schaller, J. Potratz

CHED 572. Evaluating the effect of nucleotide modifications on G-wire self-assembly. **A. Minogue**, T.C. Marsh

CHED 573. Synthesis and characterization of silver-coated gold nanoparticles as drug delivery vehicles introduced to yeast cells in vitro. **A. Alfaro**, B.D. Gilbert

CHED 574. Investigation of selective reactive oxygen species quenching ability of a novel self-cyclizing antioxidant and its derivatives. **P.A. Hahn**, S. Abdul Salam, E. Merino, J. Liu

CHED 575. Structure-function relationships in the HIV-1-Rev-Response-Element protein complex. **C. Garfola**, I. O'Carroll

CHED 576. Effect of metal ion compound concentration on the degradation of neuromelanin with application to Parkinson's disease. **B. Sutterfield**, G. Ludewick, C. Schinnerer, G. LeBlanc

CHED 577. Characterization of inhibitors of DNA-damage bypass polymerase DinB for SOS induction. **J. Andrade**, C.E. Fitzgerald, A. Hotchkiss, N.M. Antczak, S. Lone, P.J. Beuning

CHED 578. In silico Pin1 inhibitor testing: Implications towards anti-cancer drugs. **A. Yanumula**, N.A. Valley, C.W. Wostenberg

CHED 579. Kinetic studies on the aqueous chemistry of the glutathione-methyleneoxindole conjugate to model its inhibition of glyoxalase I. **A. Borges**, J. Witcher, E.J. Brush

CHED 580. Isatin thiosemicarbazone ligands and their characterization by NMR spectroscopy: Formation of their Cu(II) metal complexes. **A.K. Buckner**, J.E. Little, S.G. Bowman, X. Jiang, E.C. Lisic

CHED 581. Purifying potential cancer-inhibiting compounds in basket plant (*Callisia fragrans*). **S. Ho**, A. Bermudez, K. Truong, M. Brandon, A. Hoffman

CHED 582. Identification of the enzyme responsible for acp3U tRNA modification in bacteria. **M. Thomas**, T. Vornheder, J. Burchett, J.B. Mamaril, M. Guy

CHED 583. Effects of oxidative stress on non-B DNA structures in a yeast model system. **A. Riggs**, N. Mebane, M. Douglas, K.M. Vasquez, M. Zewail-Foote

CHED 584. Identification of tRNA 2'-O-methylation enzymes in humans and fruit flies. **R. Bales**, J.B. Mamaril, M. Guy

CHED 585. From folklore to reality: A biochemical study of the anti-carcinogenic properties of the *Annona cherimola.* **P. Cheng**, S. Deprele, L. Nogaj

CHED 586. Expression and purification of *Plasmodium falciparum* cytochrome c. H. Prieto, **Z. Wright**

CHED 587. Assembly of ASK1-MKK4/7-JNK3 kinase cascades. **R. Baker**, X. Zhan

CHED 588. Inhibition of *Borrelia burgdorferi* Bgp MTA/SAH nucleosidase. **T. Firica**, **W. Meyers**, R. Mukuna, L.

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Wayment, J.H. Thurston, D. Xu, K. Cornell

CHED 589. Understanding the generation of the non-proteinogenic amino acid β-hydroxyasparagine in bleomycin biosynthesis. **A. Vaze**, C.T. Calderone

CHED 590. Peptide-functionalized magnetically-active nanoparticles for targeted manipulation of amyloid fibrils. **N.D. Fusco**, B.D. Fellows, J.E. Smith-Carpenter, O.T. Mefford, B.J. Alper

CHED 591. Exploring the mechanism of glyoxalase I inhibition and inactivation by the glutathione conjugate with 3-methyleneoxindole. **J. Witcher**, A. Borges, E.J. Brush

CHED 592. Inhibition of oxidative DNA-protein crosslinking via tryptophan based antioxidants. **J.I. Contreras**, **A. Hernandez**, **D. Moore**, P. Perez, E.D. Stemp

CHED 593. Effect of tRNA modifications on pseudohyphal growth in yeast. **J.H. Brooks**, D. DiVita, K. Stuessel, J. Carmen, M. Guy

CHED 594. Identification of protein interactions for the mitochondrial transcription factor TFAM and mutants. **S. Reece**, M. Bestwick

CHED 595. Determining the role of retinoid X receptor alpha in mitochondrial DNA transcription. **S. Rempelos**, M. Bestwick

CHED 596. Effects of parthenolide on heat shock proteins. **T. Bailey**, **U. Dinh**, **J. Ferris**, R.E. Connor

CHED 597. Quantifying the role of copper in modifying cytochrome c oxidase expression and oxidant production in yeast mitochondria. **M.E. Walser**, M. Bestwick

CHED 598. Structural characterization of the RRE RNA of the human endogenous retrovirus K. **B. Kondrup**, I. O'Carroll

CHED 599. Design of a bifunctional nucleobase for molecular recognition of G-C base pairs in double-stranded RNA. **M. Campbell**, K. Hess, **L. MacRhyann**, C. Schweibenz, A.K. Williams, E. Rozners, T.E. Hagan, L. Gibson, J.A. MacKay

CHED 600. Fluorescent detection of reactive oxygen species in *Saccharomyces cerevisiae* applied to chronological lifespan. **K. Schultz**, M. Bestwick

CHED 601. Elucidating the role of transcription in adaptive mutagenesis with *rad26Δ* cell lines of *Saccharomyces cerevisiae*. **X. Huang**, T. Saxowsky

CHED 602. Structure-function relationships in P99 cephamycinase. **A. Sica**, S.T. Lefurgy

CHED 603. Elucidating the mechanism of action of titanium(IV) complexes for a new anticancer drug design strategy. **S. Perez**, E. Akam, K. Gaur, Y. Delgado, E. Tomat, A.D. Tinoco

CHED 604. Withdrawn

CHED 605. Utilization of the β-Glutamyl Cycle by NIH-3T3 cells. **N.S. Kowalkowski**, G. Boysen, R.B. Penney, M. Clemens

CHED 606. Impact of Cu(I) on zinc finger structure and function. **H. Phan**, C. Phan, K.E. Splan

CHED 607. Ethanol inhibition of protein synthesis in mammalian cells. **A.A. Pohl**, G.H. Purser, R. Sheaff

CHED 608. Assessment of the toxic effects of PAH on the pancreas of pregnant sprague dawley dams. **S.A. Buckeridge**, H.K. Wilson, E.W. Howerth, W. Yau, **W.E. Gato**

CHED 609. Chemical trapping of residual vancomycin to mitigate bacterial selection for resistance. **B. Russ**, R.W. Mull, Y. Tal-Gan

CHED 610. Isolation of antibacterial and antifungal activity of ancient soil sediment actinomycetes. **M. Otto**, A. Hoffman

CHED 611. Characterizing a novel signaling pathway in *Pseudomonas entomophila:* Elucidation of the signal cascade initiated by pseudomonas virulence factor (PVF) through transposon mutagenesis. **M. Knechel**, A. Kretsch, B. Li

CHED 612. Assessment of the link between environmental exposure and type-1 diabetes induction. **I. Seise**, Z.A. Pilz, W.E. Gato

CHED 613. KDAC6: Catalytic domain substrate specificity. **I. Parham**, T. Toro, T. Watt

CHED 614. Synthesis and structural variations of peptide-based molecular building blocks and their self-assembly. **A. Jeffreys**, J. Bird, L. Laperriere, D. Patterson, S.C. Butler

CHED 615. Zebrafish as a brain model to investigate the anticonvulsant properties of a photoactivatable diazepam. **W. Scudder**, J. Dallman

CHED 616. Examining longitudinal immunohistochemistry of alpha and beta cells in the NOD-mouse model of type 1 diabetes. **A. Short**, W. Joesten, M. Kennedy

CHED 617. Effect of polyphenols on buprenorphine metabolite concentrations. **A. Leddon**, M.A. Fisher

CHED 618. Effects of green tea on blood glucose levels in mice with induced diabetes. **C. Gribik**, B.A. Davis

CHED 619. Determining detection limits of gold nanospheres through UV/VIS spectrometry. **D. Daujatas**, K.E. Molter, D. Graham

CHED 620. Tyrosine 141 provides an important hydrogen bond in DNA polymerase β. **C. Westgate**, S. Lone

CHED 621. Drivers of tunable iridescence in squid skin. **C.V. Sharma**, R. Levenson, D.E. Morse

CHED 622. Effect of vitamin D_3 on paclitaxel potency in triple negative breast cancer cell lines. **C. Wilhelm**, **Z. Clor**, J. Kelts

CHED 623. Mechanistic studies of para-guaiacols as new substrates for dehaloperoxidase from *Amphitrite ornata*. **N.C. Sanders**, A. McGuire, R.A. Ghiladi

CHED 624. Expression of charged transfer species in *Sewanella oneidensis* in the presence of nanomaterial metals. **A.M. Bell**, R. Payne, S. Lampa-Pastirk

CHED 625. Spectroscopic studies of metallo-β-lactamases and inhibitors with β-Lactam antibiotics. **C.G. Miller**, A. Bergstrom, Z. Chen, A. Chen, P. Thomas, R. Bonomo, W. Fast, S. Cohen, R.C. Page, D.L. Tierney, M. Crowder

CHED 626. Using CRISPR/Cas9 system to develop switchable gene expression cassettes in *Arabidopsis thaliana*. **R. Spurlin**, C. Doherty

CHED 627. Analysis of palmitoylated actin by mass spectrometry. **J. Merritt**, L.R. Frost

CHED 628. Purification and crystallization of geranylgeranylglyceryl phosphate synthase from *T. volcanium*. **B. Gillott**, K. Alderfer, J.A. Himmelberger

CHED 629. Evolvability vs. barrel contribution to the active site in TIM barrel fold superfamilies. **A.Z. Xiang**, E.C. Mundorff

CHED 630. Electrochemical studies of L-histidine/zinc interactions in aqueous media. **D. Clark**, G.T. Cheek

CHED 631. Synthesis of giant unilamellar vesicles for use in studying the stability and permeability of cellular membranes. **C. Schweibenz**, T.E. Hagan

CHED 632. Overexpression of YAP1-TFE3/FAM118B fusion genes. **C.R. Love**, F. Szulzewsky, E. Holland

CHED 633. Deducing the mechanism by which deprenyl increases lifespan in *C. elegans*. **H. Folse**, **W. McLean**, K. Weeks

CHED 634. Quantifying tetrodotoxin using a competitive ELISA. **D. Schreiner**, R.L. McCann, P. Delis

CHED 635. Encapsulation of elastase inside the P22 virus-like particle. **K. Anazia**, D. Patterson, A. Azhgani

CHED 636. Analysis of biogenic amines present in fossilized black flies. **M. Birmingham**, M.A. Fisher

CHED 637. Examining the glutathione S-transferase assay: Understanding nitro position specificity using disubstituted chloronitrobenzenes. **Y. Olowookere**, **Q. Le**, K. Drake

CHED 638. Catecholamine compounds as inhibitors of amyloid β-42 aggregation in Alzheimer's disease. **C.V. Johnson**, S.J. Gravelle

CHED 639. Characterization of ligand binding to supramolecular G-DNA. **E. Kalb**, T.C. Marsh

CHED 640. Insights into immune mechanisms through immunoblot analysis of activation induced cytidine deaminase (AID) point mutations. **A. Malik**, J. Chaudhuri

CHED 641. Determination of the pathway leading to zonula occludin 1 phosphorylation and subsequent tight junction alteration in diabetic retinopathy. **R. Shaffer**, R.L. McCann

CHED 642. Evaluating a dissolved oxygen sensor using glucose oxidase. **D. Raval**, A. Kalantari, R. Sheaff

CHED 643. Functional cysteine residues for antigen 85C activity. **A. Mandato**, Y. Chai

CHED 644. Molecular mechanics investigation of the potential binding sites of MYCN in the treatment of neuroblastoma. **H. Foster**, M. Dorko

CHED 645. Sequential encapsulation of enzymes within the P22 virus-like particles indicates maturation of an enzyme is important to obtaining optimal kinetic activity. D. Patterson, **C. Hjorth**, A. Irias, J. Bird, T. Douglas

CHED 646. Development of a light-based dissolved oxygen sensor. **A. Kalantari**, D. Raval, R. Sheaff

CHED 647. Deciphering AMB biosynthesis. **Y. Miao**, C.T. Calderone

CHED 648. Isolation and characterization of dandelion (*Taraxacum officinale*) peroxidase. **P.A. Voss**, S.C. Silver

CHED 649. Investigation of potential drug inhibitors against DNA polymerase Eta. **K. Bryson**, S. Lone

CHED 650. EF-hands 3 and 4 have distinct roles in modulating DREAM conformations. **D. Seka**, J. Miksovska

CHED 651. L- and D- glutamine peptide synthesis: Microscale. **A. Murphy**, D. Harris

CHED 652. Development of hepatocellular carcinoma and TP73 expression: Does DNA methylation play a role? **S. Samuel**, Z. Sherif, Z. Yao

CHED 653. Analysis of cilantro and coriander extracts as natural chelates for treating mice exposed to lead acetate. **E. Volna**, B.A. Davis

CHED 654. Investigating the proteolytic processing of mitochondrial fusion protein OPA1. **K. McMahon**, **C. Griggs**, J. Fishovitz

CHED 655. Comparative analysis of the SH2B3/LNK gene in mammals: A key to understanding myeloproliferative neoplasms. **A. Adebanjo**, Z. Zhao

CHED 656. Detection of N4-acetylcytidine modification in *saccharomyces cerevisiae* mRNA. **B. Williams**, B. Addepalli, P.A. Limbach

CHED 657. Proteomic analysis of MTN deficiency in enterohemorrhagic *E. coli* O157:H7. **K.R. Bertagnolli**, M. Boll, G. Liu, S. Pu, K. Cornell

CHED 658. Water-soluble red fluorophores: Synthesis, spectral properties, and protein association study. **H. Parker**, **H.R. Lykins**, R. Choudhury

CHED 659. Study of the degradation of natural and unnatural amino acids in extraterrestrial conditions. **K.L. Davidson**, C.C. Mammoser, A.J. Gunter, S. Dhar, B. Brown, J.R. Peller, L.A. Rowe

CHED 660. NO detection with bovine oxyhemoglobin. A. Smith, **D.J. Hirsh**

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CHED 661. Effects of DMSO on uptake of polyphenols by *Escherichia coli*. **C. Cardenas**, H. Udo, K. Griffin, J. Meyers

CHED 662. Toward segmental isotopic labeling of large disordered polypeptides. **R. Cachero**, J. Antos, S. Smirnov

CHED 663. Expression of proteins TNF-β and VEGF-C involved in hepatic tumor induction of fibrosis. **M. Eichers**, D. Martin

CHED 664. Characterization of hen egg lysozyme and bovine serum gamma globulin amyloid fibrils using thioflavin T fluorescence and scanning electron microscopy. **C. Engesser**, S. Skaar, J. Welshons, M.E. Lee

CHED 665. Preventing aggregation in peptides derived from β-sheet rich sections of β -synuclein. **B.R. FItzgerald**, S. Petty

CHED 666. Biosynthesis of zinc sulfide and cadmium sulfide nanoparticles with *Shewanella oneidensis* . **S. Forney**, A.M. Bell, S. Lampa-Pastirk

CHED 667. White turnip peroxidase enzymatic stability with calcium chloride and ethylene glycol. **C. Munson**, A. Hoffman

CHED 668. Understanding origins of multicellularity by protein analysis of *Monosiga brevicollis* vinculin. **M. Delgadillo**, R.H. Singiser

CHED 669. Characterization of drug-protein interface between methylene blue and *P. falciparum* glutathione reductase using HDX mass spectrometry. H. Prieto, **C. Vazquez**

CHED 670. Comparative study of unfolding states of lysozyme and cytochrome C employing continuous-wave spectroscopy. **R. Pedretti**, S. Lampa-Pastirk

CHED 671. Development of the molecular biology and crystallization processes for fruit fly telomeric proteins. **M. Loncaric**, G. Horner, E.M. Miller, C. Brazel, R. Kurzhals, C. Ragain

CHED 672. Inhibition of luciferase by novel napthoquinone derivatives. **A. Rowe**, O.J. Alao, J.C. Dicesare, R. Sheaff

CHED 673. Effects of macromolecular crowding on the kinetics of human dihydrofolate reductase. **T. Sheehy**, D.W. Seybert

CHED 674. Conformational study of surface attached proteins by attenuated total reflection spectroscopy. **M. Hallberg**, B. Negru, H. Shi, M. Su

CHED 675. Inducing β-sheets in disordered peptides in β-Synuclein. **P. Mon**, S. Petty

CHED 676. Detecting enzyme activity in coastal aerosol. **A. Anides Morales**, M. Pendergraft, C. Lee, F. Malfatti, K. Axelrod, K.A. Prather

CHED 677. Mapping protein repertoire in the cell. **K. Cave**, T. Mithu, A. Barnes

CHED 678. Investigating the nucleating region of protein misfolding in alpha-synuclein. **C. Fernandez**, S. Petty

CHED 679. Exploring efficient methods for protein production in an undergraduate lab setting. **H. Simpson**, **A. Wilson**, J. Johnson, C.D. Mitchell, T. Dunlap

CHED 680. Effects of lipophilicity of propofol derivatives on cancer lung cell death. **J.R. Miller**, K.S. George Parsons

CHED 681. Investigating the loss of function of position 470 in human DNA polymerase K using site-directed mutagenesis. **P. Chong**, C.E. Fitzgerald, S. Lone

CHED 682. Solid phase peptide synthesis protocol optimization and application. M.J. Crawford, **B. Day**, **J.F. Larrimore**

CHED 683. Biophysical characterization of a G-quadruplex structure on the FMR1 gene at exon 12. **P. Cannanbilla**, M. Mihailescu

CHED 684. Comparative analysis of bisphenol A (BPA) versus human papillomavirus induction of oncogenic genomic instability. **E. Canty**, **S. Arya**, S. Mingarelli

CHED 685. Amino acid metabolism by cells lacking the tumor suppresser p27kip1. **R. Kaur**, R. Sheaff

CHED 686. B35 neuroblastoma cells cultured on phosphonic acid-modified and unmodified nitinol nanoparticles to test effects on neural morphology. **S. Garretson**, **L. Salameh**, H. Smith, N. Spitzer, R. Quinones

CHED 687. Differential oxygen usage in cells lacking the tumor suppressor p27kip1. **D. Thomas**, A. Saleh, R. Sheaff

CHED 688. Crystallographic studies of PrP: Discovering potential leads for drug development. **F. Pavlovici**, M. Nonato Costa

CHED 689. Conformational analysis of substrate bound methylenetetrahydrofolate reductase mutants utilizing hydrogen-deuterium exchange and mass spectrometry. E.M. Marzluff, E.E. Trimmer, **J. Wang**

CHED 690. Effect of the anti-cancer drug KP1019 on DNA in cancerous and healthy epthelial cells. **A.D. Groover**, K.L. Hayden

CHED 691. ANGPTL4 promotes lymphangiogenesis in head and neck squamous cell carcinoma. **T. Linfield**, H. Park, D. Menon, S. Montaner

CHED 692. Methionine 234 participates in orientating substrate for catalysis by human carbonyl reductase I. **J. Williams**, **M. Paul**, S. Etzler, M. Brownlee, D. Lobato, H.A. Charlier

CHED 693. Synthesis and incorporation of 1,2-alkanolamine-functionalized lysine as a non-canonical amino acid into GFP. **C. Rowlett**, J. Morse, W. Liu

CHED 694. Novel ribociclib derivative induces cell cycle arrest and cell death. **T. Hansel**, K. Barkovich, Q. Fan, K.M. Shokat, W.A. Weiss

CHED 695. Development of an unnatural amino acid-specific aminoacyl tRNA synthetase. **C.C. Mammoser**, L.A. Rowe

CHED 696. Analysis of the secondary structure of *C. parvum* pyruvate kinase and its novel disulfide bridges. **J. Potts**, K.L. Hayden, D. Chattopadhyay

CHED 697. Affect of various genetic mutants on intraflagellar transport in *Chlamydomonas reinhartii*. **M. Loncaric**, J. Lee, A. Turner, J. Kessler

CHED 698. Probing the tetrameric structure of *Leishmania major* pteridine reductase (PTR1) with point mutations and interface-derived peptides. **M.G. Johnson**, J. Gavenonis

CHED 699. Fluorescent tagging of HIV-1 using a novel recombinant protein. **D. Haas**, B. Roper, **M. Lauria**, M. Farrar, J. Kleingardner

CHED 700. Correlating the stability of coiled-coil structures with changes in the sequence. **E. Allgeyer**, P. Fisk, W. Cross, M. Blackburn

CHED 701. Development of techniques for the comparison of tetramers and dimers of MTHFR with hydrogen-deuterium exchange liquid chromatography and mass spectrometry. **A. Glebov-McCloud**, C. Jeon, E.E. Trimmer, E.M. Marzluff

CHED 702. Preparation of small laccase (SLAC) for immobilization via click chemistry and bioremediation applications. **B. Mushala**, C.M. Johnson

CHED 703. Effects of macromolecular crowding on enzyme kinetics. **C. Chung**, **J. Jackson**, **K. Slade**

CHED 704. Effect of Hierba Santa and Hierba Manayupa extractions on HeLa cells and the identification of their chemical composition via GC/MS. **A. Aceves**, C. Castillo, S. Deprele, L. Nogaj

CHED 705. Regulation of miRNA maturation pathway by pre-miRNA G-quadruplex structure. **J. Roth**, M. Mihailescu

CHED 706. Exploring intermolecular interactions during the early stages of phase separation in elastin-like proteins. **C.J. Price**, **T. Branyan**, Y. Zhang, G.L. Bidwell, J.J. Correia, N. Fitzkee

CHED 707. Cloning, overexpression and purification of tetrahydrodipicolinate *N*-succinyltransferase (DapD) from *Serratia marcescans*. **A.F. Clark**, **B.S. Lawson**, C.M. Johnson

CHED 708. Structure-activity relationship studies between GBAP analogues and the *Enterococcus faecalis* fsr quorum sensing circuit. **C. Cameron**, D. McBrayer, B. Gantman, Y. Tal-Gan

CHED 709. Preparation of the antifungal compounds HSAF and analogs from *Lysobacter enzymogenes*. **B. Lacock**, J. Jiang, L. Du

CHED 710. Effectiveness and mechanism of action of modified porphyrins for photodynamic therapy of triple negative breast cancer cells. **A. Abbott**, **H. Brandon**, J.E. Bradshaw, T.E. Hayes

CHED 711. Regulation of plant defense compound synthesis in oilseed crop *Camelina sativa* in response to biotic stress. **G. Aguirre**, J. Celenza, M. Babaei Amameh

CHED 712. Structural investigations on ER membrane complex subunit 9. **C. Murphy**, **B. Wilcox**, K.R. Gallagher

CHED 713. Analysis and characterization of lanthipeptide biosynthetic gene clusters in *Salinispora*. **M. Halbert**, **D. Scott**, C. Kittrell, E. Limbrick

CHED 714. Pulse amplitude modulation fluorometry as a means to determine photosynthetic modes of *Chlorella vulgaris*. **P.E. Adkins**, D. Kolling, B. Woodworth, A. Holland, A. Stevenson

CHED 715. Concentration dependence of TDP-43 aggregation during stress conditions. **M. Guzman Sosa**, V. Harjono, B. Zid

CHED 716. Metabolic response of cells lacking the tumor suppressor p27kip1 to low oxygen levels. **A. Saleh**, D. Thomas, R. Sheaff

CHED 717. Exploring the molecular mechanism of Tat-SF1 in HIV-1 infectivity through fluorescence correlation spectroscopy. **R. De Cataldo**, J. Trautman, K. Griffith, K.H. Fogarty, H.B. Miller

CHED 718. Using curcumin to target cancer cells with deregulated p27kp1. **J.J. Parackal**, K.M. Counter, R. Sheaff

CHED 719. Determining carbon source hierarchy of *Sinorhizobium meliloti* using ^{1}H NMR spectroscopy and complete reduction to amplitude frequency table (CRAFT). C. Hughes, N. Stubb, **D.P. Soulsby**, D.B. Wacks

CHED 720. Identification of Pks13 inhibitors for antitubercular drug discovery. **S. Leon Quinonez**, R. Shrestha, A. Aggarwal, A. Roychowdhury, M.K. Parai, W. Dong, J.C. Sacchettini

CHED 721. Kinetics of the non-enzymatic hydrolysis of aqueous l-arginine ethyl ester in vitro. **P.A. Harville**, A. Beffa, M.D. Reavis, G.H. Purser

CHED 722. Hydroxylamine reactivity with heme proteins. J. Vardanega, C.J. Krewson, **Q.C. Durfee**, B.N. Bradley, C.R. Andrew

CHED 723. Synthesis of hydroxylamine building blocks for oxime-based diversity libraries. **W. Oyewole**, D. Huang, L.E. Brown

CHED 724. Investigation of the effect of molecular weight on polymer blood compatibility. **R.O. Anyaeche**, N. Ayres, Q. Chai

CHED 725. Comparing attachment of myoglobin and BSA on nanodiamonds. **C. Sylvia**, B. Negru, H. Shi, M. Su

CHED 726. Molecular modeling of human β-glucuronidase. **A. Hawks**, K.T. Lane

CHED 727. Up-cycling expired ibuprofen. **C.N. Harris**, H.S. Barcena

CHED 728. Effects of oxidative DNA damage on survival and mutagenesis in *Saccharomyces cerevisiae* . **O.U. Egejuru**, T. Saxowsky

CHED 729. *In vivo* inhibition of *S. cerevisiae* β-glucosidase validates molecular modeling and *in silico* inhibitor docking studies. **J.L. Turner**, S.A.

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Kennedy

CHED 730. Development of *Escherichia coli* membrane preparations of human cytochrome P450 2A6. **J. Velasco**, J. Harrelson, J.M. Chan

CHED 731. Design extraction techniques of the hemolymph in invertebrate species from Puerto Rico. **S.M. Escobar Avilés**, B.J. Ramos-Santana

CHED 732. New insights into the "Manna from Heaven" hypothesis. **C. Laubenthal**, E. Shipley, J. Sebree

CHED 733. Structure-activity relationship studies of the competence stimulating peptide (CSP) signal utilized by *Streptococcus mutans*. **S.R. Hamry**, C. Bikash, Y. Tal-Gan

CHED 734. Mechanism of DNA hydrolysis and target specificity of Co, Ni, and Zn cyclen and cyclam complexes. M. Oertel, S.I. ONeal-Johnson, **A. Bond**, **P. Vahchuama**, L. Gwyn

CHED 735. Crosslinking interactions between stromal cpTatC and mature precursor. **G. Thomas**, K. Hird, A. Habtemichael, C. Dabney-Smith

CHED 736. Expressing & engineering eukaryotic lipid channels in *Escherichia coli*. **T. Zlomie**, G. Conover, A. Laganowsky

CHED 737. Quadruplex molecular beacon stability: Salt & sequence effects. **A. Brink**, C.H. Battle

CHED 738. Effects on the behavior and survival rate of *Daphnia magna* exposed to silver nanoparticles functionalized with acetylsalicylic acid. **M. Barriera Diaz**, Y. Santos Vazquez, A. Homs Ortiz, J.I. Ramirez Domenech

CHED 739. Fast detection of cancer biomarker proteins with quantum dots. **A. Rowley**, T. Parks, M. Yu

CHED 740. Regulation of the class II transactivator (CIITA) by the molecular scaffold 14-3-3 beta. **H. Malik**, D. Cressman

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Biotechnology

Cosponsored by BIOT and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 741. Paper-based lateral flow strip for detection of traumatic brain injury protein biomarker. **D. Shell**, X. Gao, N. Wu

CHED 742. Glucose and xerogel incorporated Prussian Blue modified electrochemical sensors. **A. Moreno**, D. Budner

CHED 743. Modification of collagen's surface through the attachment of histidine-tagged peptides. **J. Pham**, V. Suresh, J.A. Chmielewski

CHED 744. Ultra-sensitive assay development for early detection of tuberculosis. **M.I. Almaraz**, L. Xie, D. Walt

CHED 745. An investigation of PHLPP1 phosphorylation. **J. Shirkey**, A. Grezchnik, A. Newton

CHED 746. Maximizing output from an aspirin producing bacteria. **M. Morehart**, **B.A. Lizotte**, **M.J. Duckwall**, L. Gwyn

CHED 747. Structure-based design of molecularly imprinted polymers for G-quadruplex nucleic acids. **J.D. Mizvesky**, **R. Wodzinski**, **A. Golod**, **M.R. Elshaer**

CHED 748. Cobalt redox mediators for integration in photosystem I biohybrid solar cells. **E.A. Ooi**, J. Medina, A. Teodor, N. Brady, M. Vaughn, B.D. Bruce, J. Bergkamp

CHED 749. Structure activity studies of insulin recognition by cucurbit[7]uril. **H. Anderson**, **M. Gallagher**, W. Li, A. Grice, A.R. Urbach

CHED 750. Developing the HK97 virus-like particle as a nanomaterial platform. **M. King**, D. Patterson

CHED 751. Antifungal activity induced by generation of reactive oxygen species. **D. Little**, K. Anderson, A.G. Volkov

CHED 752. Measuring tamoxifen-inducible Cre expression in placental and embryonic tissues following treatment of pregnant female mice. **N. Popp**, M. Storage, Q. Yang, M. Bordas, R. Sood

CHED 753. Creating a DNA computer using five interconnected NAND gates with a half-adder function. **M. Grillo**, T. Molden, D. Kolpashchikov

CHED 754. Synthesis and characterization of low toxicity, ionic liquid extraction solvents. **G. Ifijeh**, R.E. Del Sesto

CHED 755. Ionic liquids as green biofuel extractants. **T. Christensen**, **A. Everett**, R.E. Del Sesto

CHED 756. Amino acid ionic liquids as non-toxic biofuel extractants. **C. Sloan**, T. Christensen, A. Everett, A.T. Koppisch, R.E. Del Sesto

CHED 757. Ionic liquid and deep eutectic materials to break down pathogenic biofilms. **T. McElroy**, **M. George**, C. Migliori, D. Warner, A.T. Koppisch, R.E. Del Sesto

CHED 758. Synthesizing carbon nano-structures. **J. Garbutt**, V. Goss

CHED 759. Characterization of eosinophils in a eosinophil-specific Notch2-deficient mouse. **D. Anketell**, **Y. Huang**, **C.L. Olbrich**, **E.W. Cornwell**, **L.A. Spencer**

CHED 760. Study of the Interactions between DNA and Metal Complexes using Surface-Enhanced Raman Spectroscopy. **J. Butkus**, S.M. Basu

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Chemical Education

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 761. Identification of Cu(II) salts based on solubility: Undergraduate laboratory experiment. **K.L. Bullard**, **J. Garcia**, L.D. Schultz

CHED 762. Investigating the mechanism and selectivities of alcohol oxidation by sodium hypochlorite: Expanding green organic chemistry lab experiments for undergraduates. S. Ellis, **T. Ellis**, T.K. Ellis

CHED 763. Investigating hazardous waste practices in the general chemistry laboratory. **O. Slater**, S.D. Wiediger

CHED 764. Withdrawn

CHED 765. Teaching the relative reactivity of carboxylic acid derivatives through a discovery-format laboratory. **L.N. Engberg**, **D. Brownholland**

CHED 766. Using molecular modeling as an aid to understanding stereoselectivity. **M. Leonhard**, A. Johnson, **D.L. Dillon**

CHED 767. Using a meta-analysis to assess the effectiveness of flipped learning in chemistry. **P. Maldonado**, A. Leontyev

CHED 768. Community Chemistry Integration Group (CCIG): Fostering an engaged community through STEM service-learning. **A. Chatters**, J. Adkins, V.C. Miles, T. McClelland, M.F. Ali

CHED 769. Instrumental and environmental chemistry discovery laboratory: Utilizing various analytical methods to study the chemistry of water. D. Vargas Trujillo, C. Grizer, R. Kidwell, J. Carvajal de Luna, S. Tittle, A. Kolek, **M. Wilk**, J.D. Beatty, M. Omary

CHED 770. Withdrawn

CHED 771. Investigating upper-division students' scientific modeling practices in the context of molecular vibration. **C. Crickmore**, J. Beck, M.N. Muniz

CHED 772. Partial least squares structural equation modeling of chemistry self-concept in introductory college chemistry. **L. Nuñez**, **C. Lai**, J. Ross

CHED 773. 3D printing in higher education. **D. Arias**, C. Arias, A. Leontyev, C. Adams

CHED 774. The development of a thermo-solvatochromism laboratory exercise for the physical chemistry laboratory curriculum. **A. Boucher**, B. Findley

CHED 775. Greener Friedel-Crafts acylation using a deep eutectic solvent: An undergraduate laboratory method. **J.R. Bonney**, I.J. Levy

CHED 776. Job's method using a diode array based spectrometer: Undergraduate experiment. **J. Lee**, R. Fietkau

CHED 777. Safety as a core value of a student chapter. **C. Wilhelm**, M.R. Wilhelm

CHED 778. Analysis of a complex gaseous mixture using ro-vibrational spectroscopy: Study of the Ira Remsen reaction for the upper-division laboratory. **T.M. Sytsma**, A. Li, J.A. Ganske

CHED 779. Design of laboratory experiences in material science and nanotechnology for cooperative project-based experimentation in general chemistry. **C. McCleary**, A. Villalta-Cerdas

CHED 780. Development of an undergraduate analytical chemistry laboratory experiment: Determination of relative fluorescence quantum yields. **P.P. Benz**, **C. Merritt**

CHED 781. Students' understandings of solution concentration. **C. Dobbs**, T.N. Abell, S. Bretz

CHED 782. Improving student understanding of intermolecular forces with transformed curricula materials. **G. Gadia**, S.M. Underwood, A.T. Kararo

CHED 783. BioVision: Object tracking in dynamic external representations. E. Shahrabani, **T.J. Bussey**

CHED 784. Improving student success on Lewis structures, VSEPR theory, polarity, and VB theory. **M. Burke**, E. Wilcox, F.M. Yarberry

CHED 785. Evaluation of potential pre-requisites in determination of student success in freshman-level chemistry courses. **J. Preston**, F.M. Yarberry

CHED 786. Improving success in freshman-level chemistry laboratories through online procedural videos. **K. Walden**, F.M. Yarberry

CHED 787. Science writing heuristic pre-lab performance compared to perceived usefulness. **N. Bonde**, D.I. Del Carlo

CHED 788. Development of a hybrid lecture/lab, interactive course in X-ray crystallography. **A.K. Kayser**, C. Bradley

CHED 789. Design of cooperative, project-based laboratory experiences to promote understanding of stoichiometry in college-level general chemistry courses. **A. Bui**, W. Fernandez, A. Villalta-Cerdas

CHED 790. Exploring connections between instructor discursive moves and student participation. **H. Fu**, M. Takemura, R.S. Cole

CHED 791. Development of a Fischer esterification experiment utlizing benchtop NMR. **M. Bansal**, A.E. Brown, H. Vail, J.L. Marshall

CHED 792. Comparing the learning outcomes in chemistry outreach between elementary charter schools and title I elementary schools. **A.M. Samani**, **M. Rosqvist**, **P. Kamath**, **R. King**, **B. Stockman**, **R.R. Burraston**, R.V. Valcarce, M. Alvarez, P.J. Iles, L.D. Giddings, N.R. Bastian, R. Holcomb

CHED 793. Symbolic and space-filling representations of a combustion reaction: General chemistry students' reasoning about bonding. **K. Ferguson**, M. Popova, S. Bretz

CHED 794. Students' understanding of atomic emission using the flame test concept inventory. **C. Spieser**, A.V. Mayo, G.H. Allen, S. Bretz

CHED 795. Quantum chemical calculations of H_2 in the ground and excited states on a spreadsheet. Y. Ge, R. Rittenhouse, J. Buchanan, B. Livingston, **M. Schimelfenig**

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CHED 796. Characterizing teachers approaches in formative assessment in chemistry classrooms. H. Sevian, **K. Caushi**, V. Dini

CHED 797. Diels–Alder reaction using a solar irradiation heat source designed for undergraduate organic chemistry laboratories. S.M. Amin, A.M. Barnes, C.R. Buckner, **J. Jones**, M.K. Monroe, L. Nurmomade, T. Pinto, S.D. Starkey, B. Agee, D.J. Crouse, D.J. Swartling

CHED 798. Development of a comprehensive interdisciplinary chemistry lab course. R.A. Kharod, K.A. Coates, **S.A. Costin**

CHED 799. Let students develop quantum chemistry for a two-dimensional world. Y. Ge, **M. Schimelfenig**

CHED 800. A 3D printed photosynthesis model. **K.A. Smiar**, J.D. Mendez

CHED 801. Chemistry and the ethic of caring: How professional development can shape teachers' attitudes and beliefs about students. **D.J. Frank**, **N.W. Spurgus**, J.M. Pratt, E.J. Yezierski

CHED 802. Students' understandings of particulate representations of elements and compounds. **L. Huff**, S. Bretz, Z. Roche Allred

CHED 803. Utilization of Excel for fast Fourier transforms: Applications in analytical chemistry education. **M. Guckavan**, G. Patterson

CHED 804. Models and modeling in chemical education: Literature and textbook review. **J. Loefer**, A. Boeck, J. Beck

CHED 805. Developing undergraduate scientists: Training scientists using storyboards. **N.N. Shaw**, S.B. Sigmann, L. Richard

CHED 806. Redesigning general chemistry: Implementation of emporium learning for enhancing basic general chemistry skills. **S.J. Blaylock**, M.A. Franks, J. Emrani, M.M. Basti

CHED 807. Measuring chemistry students' cognitive load on working memory: The development of an inventory of load-inducing topics in organic chemistry 1. **K.A. Hakim**, A. Bishop, K. Enneking, J. Nogle, E. Paulson, T. Gampp, N.P. Grove

CHED 808. Measuring chemistry students' cognitive load on working memory: The development of an inventory of load-inducing topics in organic chemistry 2. K.A. Hakim, A. Bishop, K. Enneking, **J. Nogle**, E. Paulson, T. Gampp, N.P. Grove

CHED 809. Using process oriented guided inquiry learning (POGIL) in an online general chemistry course. **K. Kubiszewski**, H. Patel, **N. Plys**, **P.L. Daubenmire**, L.C. Brazdil

CHED 810. Developing a biochemistry laboratory module: *In vitro* quantification of LDH binding affinity to nicotinamide adenine dinucleotide (NAD) derivatives. **M.E. Abel**, **J.F. Mauser**

CHED 811. Nanomaterial precursor synthesis for use in organic chemistry laboratory. **E.L. Smith**, A.J. Luca, T.S. Hughes, **L.J. Tucker**

CHED 812. Using 3D printing and Arduino technology to form a 'reaction chamber'. **C. Caldwell**, J.D. Mendez

CHED 813. Chemistry in art project: Synthesis, characterization and printmaking applications of various azo dyes. **A. Hanna**, E. Jovert, **A. Paige**, P.J. Rosado, M. Forrest

CHED 814. Analysis of an atoms first pilot at the United States Naval Academy. **O.N. Bair**, D.K. Dillner, M.A. Teichert, M.J. Schroeder, T.S. Thomas

CHED 815. Development of an effective and reproducible undergraduate experiment for the analysis of chlorogenic acid (CGAs) and caffeine in coffee through high-pressure liquid. **A. Farinas**, O. Greenwood, J.A. Schafer

CHED 816. Laboratory experiment in the preparation and analysis of poly(vinyl alcohol) self-healing hydrogels. **A.P. Hilker**, **T. Mattice**, R. Morris, M. Wentzel, P. Willoughby

CHED 817. Investigating how undergraduate general chemistry students interpret and explain everyday phenomena. **A. Sundberg**, E.E. Scott, S.M. Underwood, C. Anderson, M. KK, R.L. Matz, V. Sawtelle

CHED 818. Use of learning objects for first year chemistry students at the University of Costa Rica. **A. Fernández**, H. Arce

CHED 819. Withdrawn

CHED 820. Student reflections on test performance. W.E. Schatzberg, **S. Nielsen**

CHED 821. Embedding computing using free resources in honors general chemistry. **L. Asirwatham**, A.K. Sharma

CHED 822. Pilot investigation of zoo inquiry projects for introductory chemistry laboratories. **J. Kamitono**, D.F. Donnelly

CHED 823. Measuring science outreach effect on Title One elementary schools. **B.D. Powell**, C. Gunnell, J. Burgos, L. Hannibal, C. Anderson, M. Tsun, J. Wells, N. Alkheishali, R.V. Valcarce, P.J. Iles, L.D. Giddings, N.R. Bastian, M. Alvarez

CHED 824. pI determination of Lactate Dehydrogenase for use in an undergraduate biochemistry laboratory. **C.E. Crawford**, S. Bingaman, P.S. Biser

CHED 825. Diels-Alder reaction of β-phellandrene and p-benzoquinone as an experiment for the organic chemistry teaching lab and subsequent adduct polymerization. **J.W. Wittenberg**, T.W. Nalli

CHED 826. A cluster analysis of biochemistry students' misconceptions about enzyme-substrate interactions. **M.L. DeLuca**, K.J. Linenberger Cortes, G.H. Allen, Z. Allred, S. Bretz

CHED 827. Characterizing general chemistry students' knowledge structures about models of the atom and chemical bonding. **M. Smiley**, **B. Mulligan**, E.J. Borda, M.N. Muniz

CHED 828. Data-driven curriculum reform: Energy changes during bond making and breaking. **B. Minshall**, E.J. Yezierski

CHED 829. Educational undergraduate synthesis of N-methyl Prozac®, a precursor to the classic SSRI fluoxetine. **R. Dohoney**, S.M. Schelble, C.L. Magee

CHED 830. Increasing the safety of the rainbow flame test demonstration. **A. Rossi**, **K. Wiley**, A.J. Carroll

CHED 831. Validating the use of the SAMM survey as a formative assessment in the sixth and seventh grade science classrooms to elicit students' thinking about the particulate nature of matter. **F. Wanjiku**, C. Ngai, H. Sevian

CHED 832. Investigations of riboflavin binding protein folding through fluorescence, UV-Vis and CD thermal melt studies. **J. Tomsich**, T.A. Murray, S.L. Hemmingsen, L. Pandiscia

CHED 833. Impact of required research experience on chemistry and biochemistry undergraduates. **A.M. Ruiz**, B.L. Gonzalez

CHED 834. Development of new undergraduate polymer laboratories using organic catalysts. **M. Malley**, M.T. Wentzel

CHED 835. Shedding light on student perception of chemical exposure. **B. Blackwell**, S.D. Wiediger

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Computational Chemistry

Cosponsored by COMP and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 836. Computational studies of the O_2 binding energy and activation energy of O_2 dissociation over $M_{13}@Pt_{42}$ nanoparticle catalysts. **A. Pu**, M. Paul

CHED 837. Noncovalent interactions in networks of guanidine, urea, and water. **M.H. Byrd**, A.D. Kamischke, N. Hammer, S.A. Smith, D.H. Magers

CHED 838. Role of induction and hyperconjugation in haloacetic acids. **R. Rudisell**, E.D. Glendening

CHED 839. Minima and thermodynamic properties of a large lithium ion – Stockmayer Cluster. **G. DiEmma**, S. Kalette, E. Curotto

CHED 840. Ring polymer molecular dynamics derived from the Fourier path integral. S. Kalette, **G. DiEmma**, E. Curotto

CHED 841. Hydrogen bonding in hydrogen halide dimers. **J.J. Nysschen**, E.D. Glendening

CHED 842. Can transition state analogues be used to predict reaction enantioselectivity? Studies of organocatalytic desymmetrization of *meso* anhydrides. **E. Frank**, D.L. Kohen, G.E. Hofmeister

CHED 843. Structures and thermodynamics of a lithium atom in a mixed dipole cluster. **A. Fodor**, M.J. Hyers, D. Bierwisch, E. Curotto

CHED 844. Simulations of novel nanopost plasmonic crystal structures for SERS using FDTD methods. **A. Bigness**, J.M. Montgomery

CHED 845. B3LYP study of the dehydrogenation of ethane catalyzed by iridium and rhodium clusters. **M. Schimelfenig**, H. Jiang, R. Kato, P. Gummagatta, Y. Ge

CHED 846. Computational simulations of realkylation reactions of aged-acetylcholinesterase with quinone methide precursors. **I. Pelfrey**, R. Hopper, R.J. Yoder

CHED 847. Computational investigation of the ring-opening homo- and co-polymerizations of lactide and β-caprolactone. **D.E. Garcia**, J.M. Fritsch, B. Wilson

CHED 848. Computational studies of small heterocycles towards reactivation of aged acetylcholinesterase. **N. Yoshino**, R.J. Yoder

CHED 849. Targeted trifluoromethoxyl transfer: Lithiated alkyl reagents with nucleophilic carbon. **H. Kuramochi**, K.T. Kuwata

CHED 850. Many-body convergence of the energetic and electrostatic properties of CO2 systems. **J. Cherry**, O. Sode

CHED 851. Mechanistic examination of oxygen activation by Pt: Insertion of molecular oxygen into Pt-Me bond through light catalysis. **S.M. Loria**, J.M. Keith

CHED 852. Proteasome inhibition by selected cyclophane anticancer drugs–a computational chemistry analysis. **S. Riedel**, **G. Boothe**, C. Killer, M.D. Bezoari

CHED 853. Exploration of the molecular vibrations of small carbon dioxide clusters with *ab initio* electronic structure methods. **S. Maystrovsky**, O. Sode

CHED 854. Computational design of paradromic molecular rings: n^{th} order Moebius metallacycles. **A. Goldberg**, **N. Tabassum**, M.M. Francl

CHED 855. All that glitters is gold: Modeling catalysis of hydride shifts. **S. Dutton**, C.H. McCulley, D.J. Tantillo

CHED 856. Theoretical circular dichroism spectra of β-helical proteins with the dipole interaction model including the n-π* transition. **F.N. Ngassa**, A. Jungong, I. Uporov, R. Nori, K. Thomasson

CHED 857. Computational analysis of ro-vibrations in vinyl alcohol and the formation of 2-chloroethanol. **R. Soliday**, I. Sumner, P. Raston

CHED 858. Coarse-grained predictor of protein pK_a values. **C.D. Pauplis**, J. Cvitkovic, E. Theodhori, G. Kaminski

CHED 859. Molecular drug docking on dopamine and cannabinoid receptors. **A. Walker**, U. Okafor

CHED 860. Deviations from ideality: Quantum cluster equilibrium theory and the methanol-benzene binary mixture. **N. Vigilante**, A. Buczek, M. Broda, T. Kupka, A. Kelterer

‡*Cooperative Cosponsorship*

CHED 861. Comparison of charge density to pKa for cyclic carbonyl systems. **S. Bentz**, A. Grushow

CHED 862. Computational study of the Julia-Kocienski methylenation of acetone using DFT. **M. Korman**, J. Beck

CHED 863. Theoretical studies of interactions between planar $C_{16}N_{12}$. **M.K. Alsarraj**, J. Song

CHED 864. Experimental and computational analysis of activation parameters for non-enzymatic hydrolysis of l-arginine ethyl ester at various pH values. **A. Beffa**, M.D. Reavis, P.A. Harville, G.H. Purser

CHED 865. Calculation of bond dissociation energies of electronically different N,N-dihalogenated sulfonamides. **L.J. Schroeder**, M.D. Hopkins, G.H. Purser, A.A. Lamar

CHED 866. Computational investigation of the thermal stability of protein-small molecule complexes. **K.W. Melton**, K.E. Johnson

CHED 867. Free energy study of the Diels-Alder reaction of isoprene and acrolein. **K. Gallo**, V. Roytman, D.A. Singleton

CHED 868. Molecular modeling of amphipathic molecules at an organic/water interface in the presence of divalent cations. **T.B. Martin**, K.E. Johnson

CHED 869. Investigating the thermal-stability of bacteria based alpha-amylases with molecular dynamics. **N. Olowo**, K.E. Johnson

CHED 870. Characterization of the mass spectra energetics of butane and propanol derivatives via *ab initio* methods. **A. Burke**, G. Saliba, B.B. Magers

CHED 871. A TD-DFT study of two fluorescent medical dyes. **J.A. Flack**, J.D. Alia

CHED 872. Rovibrational quantum chemical analysis of c-C_3H_2: Overcoming the failure of correlation for out-of-plane motions. **C.M. Novak**, R.C. Fortenberry

CHED 873. Characterization of amino acid based macromolecular assemblies with molecular modeling. **A. Billiot**, Y. Fang, K.F. Morris

CHED 874. Allosteric mechanism of peptide release in the molecular chaperone Hsp70. **J. Williams**, D. Merz, R.I. Dima

CHED 875. Computational studies of intramolecular charge transfer compounds. **V. Manam**, **C. Crider**, J. Song

CHED 876. Thermodynamic mechanism for the loss of CH_3SH from protonated methionine. **D. Devore**, J. Johnston

CHED 877. Withdrawn

CHED 878. Metal+ligand redox cooperativity in cobalt-catalyzed reactions. **K.G. Lopez**, T.R. Cundari, B. Gary

CHED 879. Computational investigation of the pseudo-Jahn-Teller effect on malonaldehyde and cyclobutane. **D. Zweerink**, J.N. Woodford

CHED 880. Development of phosphorylated amino acid parameters for AMBER-FB15. **J. Stoppelman**, L. Wang

CHED 881. Ammonium ligand binding to dibenzo-18-crown-6 in solvent. **B.M. Tilson**, B.B. Magers, B. Minofar, D. Reha, J. Carey

CHED 882. Theoretical investigation of isomers of C_2N_4, C_2O_4, and $C_2N_2O_2$. **D. Corey**, J. Song

CHED 883. Quantum roaming dynamics on model double Morse and ion-dipole potentials. **L. O'Connor**, Z. Kramer

CHED 884. Exploring the additivity of urea and anion interactions. **J.A. Edwards**, J. Ellenbarger

CHED 885. Thermochemical and structural properties of cyclic nitramine compounds. **J. Pina**, K.R. Jorgensen

CHED 886. Node development, movement, and dissipation in the complex plane: Utilizing numerical analytic continuation and the complex plane to understand wavepacket scattering. **J. Mosely**, C.W. Lechak, D. Bateman, B.A. Rowland

CHED 887. Exploring the oxidative carbon-carbon cleavage of ketones mediated by biomimetic models of the Ni-ARD active site. **J.B. Lumpan**, T.D. Shepherd, S.A. Toledo

CHED 888. Electronic structure calculations for lithium- and copper-containing quaternary diamond-like semiconductors. **A.N. Radzanowski**, C. Barton, J.R. Glenn, J. MacNeil, J.A. Aitken

CHED 889. First principles modeling of gaseous molecules diffusing through graphene pores. **C. Celani**, J.A. Keith, Y. Basdogan

Section H
ErnestN. Morial Convention Center
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Undergraduate Research Posters

Environmental Chemistry

Cosponsored by ENVR and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 890. Aptamer-based biosensor for the electrochemical detection of arsenite in water. **N.A. Rivera Fuentes**, K. Vega-Figueroa, P.E. Cruz Tato, E. Nicolau

CHED 891. Estimating changes from legalization of cannabis use through wastewater-based epidemiology. **R. Rushing**, J. Sadetsky, R. Carpenter, D.A. Burgard

CHED 892. Potentially toxic elements in urban soils from Lagos, Nigeria. **K. Burke**, E.I. Obolo, C. Davidson

CHED 893. Analysis of wastewater samples for attention deficit hyperactivity disorder (ADHD) medications by liquid chromatography-tandem mass spectrometry (LC-MS/MS). **W. Parker**, T.H. Boles

CHED 894. Manganese toxicity and bioaccumulation in *Chlorella vulgaris*. **N.L. Perry**, A. Smythers, D. Kolling

CHED 895. Seasonal comparison of photocatalytic degradation of tetracycline in bovine wastewater. J.E. Boyd, **P.A. Skerratt**, K. Squiggins, T.R. Hayden

CHED 896. Bioremediation of fracking waste reservoirs. **C. Fogg**, C. Cash, K. Drake

CHED 897. Metal modification for the photocatalytic degradation of tylosin and tetracycline. **M. Clothier**, **J.L. Butler**, J.E. Boyd

CHED 898. Determination of heavy metal uptake in plants grown in agar by X-ray fluorescence (XRF). **E. Lee**, M.J. Schroeder

CHED 899. Survey of microplastic pollution in surface and drinking water using FTIR spectroscopy. **N. Blackmon**, C.D. King

CHED 900. Applications of a student-centered method for the study of lead in soil through analytical chemistry. **L.M. Nitti**, C.R. Pulliam, J. Crandall

CHED 901. Nutrient processing and storage in agricultural streams and ponds as reavealed by high frequency observation. **C. Brunet**, A. Graham

CHED 902. Variation in sediment nutrient concentrations in an urban-mangrove ecosystem, Piñones, Puerto Rico. **J. Rivera Cruz**, D. Ogurcak, T. Barreto, M.V. Santos, J. Kominoski, T.A. Crowl, J. Fourqurean, M. Ross, J. Meeder, J. Smoak, A. Lugo, M. Yu, S. Charles, A. Chappel

CHED 903. Detecting nitrate with chemical field-effect transistor sensors. **J.M. Fehr**, S. Fontenot, M.M. Haley, D.W. Johnson

CHED 904. Impacts of Hurricane Harvey on distribution of metals in Greater Houston. **S. Christnacht**, E. Opperman, K. Kim, S. Das, S. Chellam

CHED 905. Impacts of cleaning agents and fouling on ageing of reverse osmosis membranes employed for potable water reuse. **R. Coker**, B. Abada, S. Chellam

CHED 906. Examination of possible lead and copper in local drinking water. **A. Trouten**, A. Bowen, M.E. Railing

CHED 907. Photolysis and biological activity of the polycyclic musks tonalide and galaxolide. **C. Heiling**, B.G. Anderson, H.A. Cumbe, J.J. Willour, A.J. Borgerding, D. Martinovic-Weigelt, K.H. Wammer

CHED 908. Catalytic hydrodefluorination of fluoroarenes and pharmaceuticals. **G. Lindquist**, A.M. Luke, T.J. Dick, A.A. Peterson

CHED 909. Preparation for service project by enviromental chemistry course: Pilot of microwave lead extraction method. **M.E. Hogue**, **P.T. Kasunic**, S.A. Radford

CHED 910. Electrochemical oxidation of brilliant green in aqueous solution. **S.A. Mayo**, G. LeBlanc, R. Sheaff, G.H. Purser

CHED 911. Urban and rural phosphorus contributions of the Pinnebog River Watershed to Saginaw Bay. **P.T. Braman**, E. Griswold, A. Rambow, A. Yankley, M. Dobulis, L. Koski, D.S. Karpovich

CHED 912. Kinetic studies of hydroxyl radical reactions with aqueous-phase methylglyoxal and glyoxal in atmospherically relevant conditions. **C. Oman**, C.M. Strollo

CHED 913. Multi-decadal assessment of heavy metals in body tissue and vibrissae of select North Pacific marine mammals. **E. Pope**, **T. Juneja**, P. Ferdinando, D.G. Giarikos, A.C. Hirons

CHED 914. TRP channel agonists in air pollutants: Possible molecular mediators of pathogenesis for environmentally-sensitive respiratory diseases. **A. Scott**, C. Deering-Rice, C. Reilly

CHED 915. Measurement of lead and zinc in plants and soil around Silver Moon Mine in Branson Creek, Missouri. **S. Montoro**, K.E. Garrison

CHED 916. Investigating the antimicrobial activity of humic acids. **M. George**, D. Warner, G. Chilom

CHED 917. Determination of copper and iron concentrations in soil samples from various locations in middle Georgia. **S. Stephenson**, **S.C. Wilder**, R. Fietkau

CHED 918. Correlation study between particulate matter and PAH concentrations through the bio-monitoring of pine tree leaves. **R. Moran**, S. Cortez, S. Deprele

CHED 919. Application of biochemical polymers in sorption of crude oil. R. Srinivasan, **M. Meadows**

CHED 920. Bioremediation of analysis group I heavy metal cations in freshwater systems. **V. Rodriguez**, C. Cash, K. Drake

CHED 921. Understanding water source contribution in urban stormwater. **D. Read**, M. Smith, J. Kominoski

CHED 922. Use of plant based polymers as effective removal agents of solid and radioactive waste in Dockum aquifer. R. Srinivasan, **T.B. Roberson**, W.M. Grumbles, **P. Naran**, **R. Olivo**

CHED 923. Identification of heavy metal in water used for agriculture in the west region of Puerto Rico. **P. Garcia Torres**, B.J. Ramos-Santana

CHED 924. Optimization of EDC detection in aquatic environments: LC-MS/MS detection & quantification of trenbolone. **A. Atwood**, S. O'Brien, C.J. Monceaux

CHED 925. Removal of organic dyes from aqueous solutions using Fe_3O_4 nanoparticles using a modified Fenton process. **C. Torres-Martinez**, C. Osorio-Cantillo

CHED 926. Analysis of nutrient concentrations and distributions in tree leaves from Costa Rican lowland tropical forests. **A. Schwarz**, J. Sager, R.L. Sanders

CHED 927. Examination of atmospheric perchlorate response during large volcanic eruptions using an Antarctic ice core. **H. Przelomski**, T. Cox, J. Kennedy, J. Cole-Dai

CHED 928. Withdrawn

CHED 929. Kinetics of methylene

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blue adsorption on humic acids. **K.A. Monday**, O. Ruiz, G. Chilom

CHED 930. Analysis of DDT and its metabolites in polluted sediment. **J. Wright**, M. Hopko, J. Liebens, **P.P. Benz**

CHED 931. Determination of heavy metal contents by atomic absorption spectroscopy (AAS) in medicinal aquatic macrophytes. **W. Figueroa**, **J. Dumeng**, Y. Cortes, **V. Rivera**, M.L. Ramos

CHED 932. Analysis of air and water samples for the presence of heavy metals in Clark County, Arkansas. **A. Eckerstorfer**, **K. Nordengren**, B.A. Rowland, D. Bateman

CHED 933. High-resolution mass spectrometry analysis of procured polyethylene extractions. **M. Brown**, A. Ter Halle

CHED 934. Challenges of hydrophosphinylation during surfactant synthesis. **V. Lee**, S. Deprele

CHED 935. Quantifying the response of model bacteria *Shewanella oneidensis* grown in the presence of plastic and plastic additives. **L. Fawcett**, M.A. Maurer-Jones, K. Koval

CHED 936. Intake of copper into *Brassica juncea* and distribution of copper in soil at various pH levels. **E. Garbioglu**, J. Bayline, J. Kilgore

CHED 937. Characterizing dissolved organic matter in surface waters through excitation-emission fluorescence spectroscopy and parallel factor analysis. **C. Vergil**, S. Pribil, K.J. Sorauf

CHED 938. Chemical and physical characterization of water quality in Wolf Creek as affected by the Lawton, Oklahoma community. C.D. Bryan, C. Iluno, **G. Jensen**, **E. Momoh**

CHED 939. Quantifying the properties of hydrocarbon mixtures containing compounds with low cetane numbers to assess their impact on diesel combustion. **S.L. Graft**, T.R. Johnson, D.J. Luning Prak

CHED 940. Determination of lead content in local water sources by differential pulse stripping voltammetry. **G. Stelmacovich**, G.D. Claycomb

CHED 941. Photocatalytic destruction of endocrine disrupting chemicals. **C. Cervantes**, J. Parsons, H.M. Morales

CHED 942. Removing lead from water with chitin and chitosan. **S. Baumgartner**, J.D. Mendez

CHED 943. Withdrawn

CHED 944. Quantification of soluble ions in atmospheric particulate matter using ion chromatography. **P.R. Tumminello**, M. Cassingham, G. Featherston, H. Dana, C.D. Hatch

CHED 945. Proposed teaching lab and improved procedure for the removal of molybdenum and sin from waste generated by the quantitative analysis of phosphate: Verification by atomic absorption spectroscopy. **M. Wood**, R. Mauldin

CHED 946. Qualitative analysis of PM2.5 organic compounds in Conway, Arkansas. **M. Cassingham**, G. Featherston, H. Dana, J.C. Gann, C.D. Hatch

CHED 947. Use of XRF as a method to study environment changes along the Upper Mississippi and St.Croix Rivers. **R.E. Schellinger**, K. McMahon, T.D. Levine

CHED 948. Water adsorption on volcanic ash as a function of relative humidity. **M. Sipes**, M. Cassingham, H. Dana, G. Featherston, C.D. Hatch

CHED 949. Effect of pH on the absorbance and structure of compounds within atmospheric aerosols. **R. Holappa**, M.M. Galloway

CHED 950. Photochemical aging of atmospheric aerosol in a diurnal cycle. **J. Ackendorf**, D.N. Grace, M.B. Sebold, M.M. Galloway

CHED 951. Effect of pH on the photocatalytic activity of PMMA-titania composite materials. **J.M. Van Riper**, E.R. Bishop, J.E. Boyd

CHED 952. Antimicrobial compounds produced by endophytes isolated from yellow rabbitbrush. R. MacKay, **M.D. Halling**

CHED 953. *Rubus ursinus*: The search for novel antimicrobial compounds. **J. Lindow**, **M.D. Halling**

CHED 954. Utilizing structure activity relationships to determine binding capabilities & selectivity in aqueous solution. **J. Sadio**, C. Fournier, S.G. Tajc

CHED 955. Novel biologically active compounds produced by endophytes from a raspberry plant. **A. Matkovska**, M.D. Halling

CHED 956. Structural-activity relationship of group 2 metal cations using pyridine based small molecules. **D. Painter**, C. Jones, S.G. Tajc

CHED 957. Refinement of the RSIT method. **S.R. Thompson**, A.S. Frantzen, M. Tiller, B.P. Oswald

CHED 958. Fluorescence based monitoring of sewage inputs to urban rivers. **L. Mendoza**, N. Mladenov

CHED 959. Analysis of methylmercury concentrations of *Morone saxatilis* in Lake Cumberland, KY show levels much greater than FDA reported values for the species. **H.D. Ellis**, E. Guth, S. Pearish, C. Chen

CHED 960. Deliquescence relative humidity of inorganic aerosols in the presence of soluble organics. **C. Merritt**, C.M. Strollo

CHED 961. Biochemical and metabolomic profiling of Switchgrass (*Panicum virgatum*), a native plant, for potential as a phytoremediation agent to clean-up BPA contaminated systems. **A. Harford**, J. Murphy, A.K. Merrill, S. Joseph, C. Roote, B. Brown, D. Giacherio, S. Zamule, P. Das

CHED 962. Lead (Pb) concentrations in households: A survey. **A. Lieberman**, F.M. Dunnivant

CHED 963. Development of magnetic iron-oxide polymer coated core-shell nanoparticles for the removal of fecal bacteria from contaminated water samples. **M. Wild**, A. Deckert

CHED 964. Reaction products of methylglyoxal and glycolaldehyde in secondary organic aerosol mimics. **D.N. Grace**, J.M. Ackendorf, M.M. Galloway

CHED 965. Developing a sustainable zero-waste multi-process remediation technology, involving chemical immobilization and phytoremediation to remove excess nutrients from a sewage treatment plant (STP) effluent. **F.E. Downes**, G. Connors, J. Murphy, I. Gergi, J. Losee, J. Wessel, D. Painter, P. Das, S. Zamule, D. Giacherio

CHED 966. Determination of biofouling mechanisms of single and binary protein solutions of BSA and hemoglobin under varying pH and salinity conditions. **S.V. Tewari**, E.M. Stennett

CHED 967. Understanding the solvent reactions of some common chloroformic acid esters with herbicidal properties. **O. Mahmoud**, **J.J. Wirick**, M.J. D'Souza

CHED 968. Iron welding fumes: Human health consequences and potential beneficial reuse. **A. Yang**, T. Luxton, J.G. Clar

CHED 969. Caffeine as an indicator of wastewater volume in rivers. **C. Wheeler**, F.M. Dunnivant

CHED 970. Comprehending the substituent and solvent effects in ethyl esters of chloroformic acid. **M.I. Dina**, M.J. D'Souza

CHED 971. Wasted fracking water: An examination of components by instrumental methods to assess potential environmental impact. **S. Wappes**, **S.M. Williams**, S. Tittle, T. Nguyen, B. Overton, D. Steffey, M. Wilk, M. Omary, J.D. Beatty

CHED 972. Pore size and zeta potential effects on colloid removal by clean microfiltration membranes. **S. Wilson**, K. Kim, H. Nouri, R.E. Baltus, S. Chellam

CHED 973. Bromination and chlorination kinetics in natural waters: How useful are data collected in "clean" systems? **M.H. Schammel**, T.L. Swanson, R.P. Dias, J.D. Sivey

CHED 974. Exploring the bromination kinetics of anisole and salicylic acid in natural waters. **T.L. Swanson**, M.H. Schammel, J.D. Sivey

CHED 975. Evaluating freshwater ecosystem quality using bioindicators and physicochemical indicators. **R. Davila-Rivera**, B.J. Ramos-Santana

CHED 976. Characterization and quantification of phosphorus containing compounds in algae biofuel. **E. Timmel**, D.S. Heroux

CHED 977. Sulfur and iron geochemistry in the rhizosphere of wild rice (Zizania palustris). **K. Lugo**, A. Orloff, S. La-Fond, N.W. Johnson

CHED 978. Release of ZnO nanoparticles used in surface coatings: Effects of NP size on leaching characteristics. **S. Boggins**, T. Luxton, J.G. Clar

CHED 979. Primary production is greener on the other side: Influence of hurricanes on the West Florida shelf. **C. Nickel**, R. Masserini

CHED 980. Modeling of surface area and pore volume of activated carbons prepared from renewable and low cost precursors. **A. Balesano**, **C. Domville**, **A. Schwartz**, **K. Seferi**, **E. Alkhatib**, P.A. Snetsinger

CHED 981. Investigation of the impacts of indirect photolysis on select contaminants along the St. Louis River. **Q.T. Whiting**, J.A. Herrli, S. Berg, C.K. Remucal, K.H. Wammer

CHED 982. Environmental fate of the steroid trendione: nucleophile effect on photochemical stability and product formation. **M. Hankard**, K.C. Breuckman, N.C. Pflug, D.M. Cwiertny, K.H. Wammer

CHED 983. Total alkalinity trends and troubles in Tampa Bay. **J. Vargas**, K. Yates, R. Masserini

CHED 984. Environmental analysis of the persistent metal pollutants from acid mine drainage using ICP-OES. **S.M. Vaal**, S.M. Lamos

CHED 985. Determination of caffeine in water sources in Morehead, Kentucky. **S. Little**, M.C. West, B.D. Miller, B.G. Vanness

CHED 986. Buoyant photocatalyst used for the degradation of organic pollutants. **K.a. Steward**, M.J. Nee

CHED 987. Optimizing the extraction and LCMS analysis of emodin for application to biological systems. **K.R. Chao**, J. Piatt

CHED 988. Investigating the green claims of bio-based plastic by measuring chemical migration during simulated food contact. **S. Virgen**, A. Burns, L. Smith, J. Layshock

CHED 989. Characterization of thiamethoxam removal from aqueous solution by select bacterial species under laboratory conditions. J. Widmer, A. Merrill, R. Pacella, **E. Hyde**, B. Biswa, J. Murphy, P. Das, S. Zamule

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Geochemistry

Cosponsored by GEOC and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 990. Withdrawn

CHED 991. Identification of adsorption sites for nucleobases on clay mineral surfaces. **H. Kats**, D. Roznovjak, R.L. Sanders

CHED 992. Investigating the impact of floating oyster aquacultures on carbon and nitrogen flux with the sediment for potential use in nitrogen-removal. **P. Dunn**, **E. Gibeault**, **K. Paquette**, D. Stone, S. Lott, R. Cox, J. Shea, R. Bence, A. Cobban, C. Mazur, V. Edgcomb, D. Rogers

CHED 993. Analyzing heavy metal contamination of abandoned cobalt mine

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in Chatham, Connecticut using handheld XRF. **L. Thompson**, B.L. Westcott

CHED 994. Advancing the vanadium paleoredox proxy: Defining the chemistry controlling vanadium speciation in sulfidic natural waters. **P. Vue**, A.A. Vezina, S. Miller, M. Casperson, T.P. Vorlicek

CHED 995. Microtopographic control of groundwater geochemistry and Hg methylation in a river floodplain. **A. Wadle**, A. Graham

CHED 996. Mercury methylation and bioaccumulation in an Iowa terrace-fen complex. **K. Smith**, A. Graham

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Green Chemistry & Sustainability

Cosponsored by CEI and SOCED
Financially supported by GCI: ACS Green Chemistry Institute
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 997. Preliminary investigation into unintended consequences of caffeine exposure on children. **J. Kinyua**, E.J. Brush, C.D. King

CHED 998. Electrochemical oxidation in wastewater samples. **L.D. Rivera Cubero**, C. Rusinek, G.M. Swain

CHED 999. Catalytic oxidative dehydrogenation of light alkanes: Energy-efficient means of meeting the demand for alkenes. **K.L. Lawrence**, M. Julin, C.A. Carrero

CHED 1000. Gas-phase partial oxidation of natural gas blends in a tubular-flow reactor. **A. Nguyen**, **N. Penaloza**, E.B. Ledesma

CHED 1001. Sustainability and cost reduction efforts in our school by converting spent cooking oil into biodiesel: Process development study. **C. Luong**, **A. Tran**, E.B. Ledesma

CHED 1002. Hydrosilylation of highly functionalized alkenes catalyzed by Pt(0) nano-dispersed in organically modified silicates. **B.R. Adolph**, **E.N. Akeroyd**, S.V. Bhatt, S.V. Bhatt, J. Fotie

CHED 1003. Synthesis of cofacial perylene bisimide luminophores for light management. **T.M. Nakama-Fukuhara**, J. D'Amelio, T. Kowalczyk, D.L. Patrick, J.D. Gilbertson

CHED 1004. Green chemistry synthesis of primary amides using microwave energy. E.A. Nalley, **T.S. Nwaiwu**

CHED 1005. Withdrawn

CHED 1006. Substituting ordinary Portland cement with biomass ash: Greener way to make concrete. J. Lynam, T. Garrett, **J.A. Supple**

CHED 1007. Synthesis and substrate testing of a bis(diphenylthiophosphinoyl) methanediide platinum(II) pincer complex for the catalytic synthesis of lactones and lactams. **A. Esper**, A. Pujol, M. Boutignon, N. Mézailles

CHED 1008. Synthesis of 1-acetyl-1-cyclohexene using ionic liquids. **B. Gillott**, **B.A. Dierolf**, F.C. Mayville

CHED 1009. Synthesis using solar irraditon and spectral analysis of meso-tetraphenylporphyrins. **T. Pinto**, G.A. Mullins, D.J. Swartling

CHED 1010. Effects of varying electrolytes in dye-sensitized solar cells (DSSCs). **J. Delgado**, L.C. Klein

CHED 1011. Synthesis of PSLA-mPEG-550: Designer surfactant for optimizing micellar catalysis through an immobilized proline-derivative catalyst. D. Brownholland, **A.J. Szczodrowski**

CHED 1012. Synthesis of a model compound for lignin and investigating catalysts for depolymerization. **M. Tan**, J. Jennings, A.K. Franz

CHED 1013. Task-specific ionic liquid as a base catalyst and a reaction medium for Michael addition reactions. **K. Akselrod**, R.N. Manchanayakage

CHED 1014. Electrophilic addition to alkenes in ionic liquids. **M. Ohlhausen**, R. Kroeker Sachs

CHED 1015. Ring opening of chalcone epoxides in a Lewis acidic ionic liquid via intramolecular Friedel-Crafts alkylation. **A. Canfield**, R.N. Manchanayakage

CHED 1016. Synthesis and characterization of a cesium-doped, iron oxide photocatalyst. **H. Li**, L.R. Sharpe

CHED 1017. Micelle-catalyzed metathesis reactions in-flow. **M.K. Jones**, D. Brownholland

CHED 1018. Synthesis of alkene-terminating steroidal surfactants designed for micelle-catalyzed organic synthesis. J. Haggett, **A.E. Reiter**, **L.N. Engberg**, D. Brownholland

CHED 1019. Greener synthesis of dithiocarbamates. **I. Hammer**, E.C. Sylvester, R.A. Haley

CHED 1020. Use of a microwave reactor to synthesize isoxazoles. **N. Aoki**, S. Helm, L. Bastin

CHED 1021. Using C-D vibration to study CO_2-ionic liquid interactions. S. Dutta, **I. Williams**

CHED 1022. Ionic liquid property effects on the natural fiber welding process. **R. Chung**, D.P. Durkin, S. Park, L.M. Haverhals, H. De Long, P.C. Trulove

CHED 1023. Green synthesis of dithiocarbamates. **G.W. Bell**, J.F. Fuller

CHED 1024. Methane reforming with carbon dioxide to produce syngas over Ni/SBA-15 catalysts. **C. Boyd**, Z. Bao, J. Dou, F. Yu

CHED 1025. Green synthesis and analysis of imine-metal complexes. **A.L. Gaynor**, J. Bennett

CHED 1026. Evaluation of imine synthesis in a variety of solvents. **J. Marcantonio**, J. Bennett

CHED 1027. Electrochemical synthesis of urea derivatives with carbon dioxide in ionic liquids. **C. Le**, Z. Huang, Z. Wang

CHED 1028. Getting insights on the influence of inorganic metal species on the activity/selectivity of HZSM-5 during CFP of pinewood towards arene compounds. **N. Stephens**, R. Thakur, C.A. Carrero

CHED 1029. Electrochemical reduction of CO_2 to CO catalyzed by superoxide radicals in ionic liquids. **M.L. McNeil**, Z. Huang, A. Gupta, Z. Wang

CHED 1030. Green synthesis of a cross-linked polymerized hydrogel containing NDHGA-capped gold nanoparticles for skin lesion treatment. **E. Rugutt**, M.O. Montes

CHED 1031. Green modifications to the Hajos pathway to an important steroid intermediate. **C. Cooper**, J.K. Berch

CHED 1032. Cyclic asymmetric aldol additions and dehydrations in hot pressurized water. **O.V. den Besten**, J.K. Berch

CHED 1033. Lipid extraction of wet algal biomass via osmotic shock. **A. Ansari**, A.M. Parker

CHED 1034. Greener options in the chemistry classroom: A titrimetric analysis of coffee. **T. Avery**, M.D. Garrett

Section H
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Undergraduate Research Posters

Inorganic Chemistry

Cosponsored by INOR and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 1035. Development of new cobalt(I) pincer complexes for catalytic applications. **S. Parkins**, Y. Li, H. Guan

CHED 1036. Ti(Deferasirox)$_2$, a highly cytotoxic chemical transferrin mimetic Ti(IV)-based compound, displays one of the highest aqueous stabilities in the Ti(IV)-based anticancer field. **A. Vazquez**, S.A. Loza-Rosas, A. Vazquez, K.I. Rivero, L.J. Negrón, Y. Delgado, J.A. Benjamín-Rivera, T.B. Parks, C. Munet Colón, A.D. Tinoco

CHED 1037. Cross-linking investigation of recycled poly (vinyl chloride) with recycled cross-linked polyethylene (XLPE mesh #50). **R.O. Ali**, S. Soares, N. Hnatchuk, W. Brostow

CHED 1038. Analysis and characterization of iron, manganese, and cobalt catalysts for oxidation of a lignin model compound. **G. Perry**, K. Aletty, E. Brown, K. Young

CHED 1039. Investigation of the inclusion complexes of alpha-cyclodextrin with anthranilic acid-derived N, N, O-terdentate ligands. **G. Reinartz**, N.R. Lien

CHED 1040. Synthesis and characterization of transition metal lanthanide metal-organic materials. **V. Parra**, M. Payne, A.S. Jayasinghe, T. Forbes

CHED 1041. Development of water-soluble photodynamic therapy agents. **S. Owens**, J.E. Bradshaw

CHED 1042. Indium phosphide etching mechanism studies. **J.M. Rosado**, E.J. McLaurin, S. Lee

CHED 1043. Synthesis and reactivity of carboxylated CB_{11}^- carborane anions. **W.T. Mendelsohn**, G. Dwulet, J. Reed, M.A. Juhasz

CHED 1044. Synthesis, characterization and spectroscopy of a terbium-centered complex: Remarkable emission from a colloidal mixture. **A. Daniels**, L.A. Ligon, J.J. Stace

CHED 1045. Mechanical and photochemical properties of polysaccharide-based, metal-coordinated hydrogels. **J. Medina**, A. Ostrowski

CHED 1046. Silylation of pyridine and pyridine derivatives using diruthenium catalysts. **J. Prybil**, R.M. Chin

CHED 1047. Precipitation of metal-organic frameworks at elevated temperature. **J.A. Daly**, X. Chen, J.B. Parise

CHED 1048. Spiro synthesis for uses in perovskite solar cells. **D.W. Valencia**, J. Potvin, J. Herring, S.K. Hurst

CHED 1049. DFT study of $[Co_4O_4]$ clusters relevant to O_2 formation by water splitting. **K. Pasley**, C.A. Bayse

CHED 1050. Luminescence of lanthanide/transition metal heterobimetallic phosphinoamide complexes. **A.T. Haley**, K.A. Burke, A. Hill

CHED 1051. Compounds containing the anionic half-sandwich (pentamethylcyclopentadienyl) vanadium(III) chloride complex, $[Cp^*VCl_3]^-$. **H.J. Bates**, **B. Vo**, **N.E. Wyse**, C.D. Abernethy

CHED 1052. Kinetics and product characterization of the oxidation of veratryl alcohol catalyzed by an iron coordination complex. **E. Brown**, K. Aletty, G. Perry, C. Apel, C. Alsip, L. Niu, K. Young

CHED 1053. Polymerization and metal coordination of spirane complexes for material studies. **J. Potvin**, D.W. Valencia, J. Herring, S.K. Hurst

CHED 1054. Synthesis, characterization, and photosensitization of a series of $[Ru(LL)_2(quo)]^+$ complexes as potential PDT agents. **F. Delano IV**, **K. Roche**, D. LaChance, B.M. Bailey, R.N. Garner, B.B. Sears

CHED 1055. Hydration of nitriles to amides using silver trifluoromethane complexes. **W.J. Cochran**, B. Fox

CHED 1056. Synthesis and characterization of a bipyridine adduct for the formation of new Ru(II) complexes. **A. Chung**, D.G. Giarikos

CHED 1057. Solvent-dependent photophysical properties of luminescent metal-organic frameworks doped with polypyridyl osmium carbonyl complexes. **K. Hess**, J.A. Rood, K. Kneas

CHED 1058. Exploring the potential of biogenic chelidonic acid as a trigonal building block for mixed-metal MOFs. **T.B. Tyson**, J.F. Eubank

CHED 1059. Toward metal-organic

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frameworks containing isocyanoarenes and half-sandwich iridium(III)-based building blocks. **T. Stell**, J.J. Meyers

CHED 1060. Raman and FTIR spectroscopy of tooth enamel and dentin. **C. Hueske**, **S. Marazita**, M.B. Jacobs

CHED 1061. Synthesis and characterization of $LaMnO_3$ perovskite-based catalysts. **R.R. Mitton**, J.M. Garcia-Vargas, M.A. Tarr, A. Giroir-Fendler

CHED 1062. Systematic investigation into the bonding, electronic structure, and reactivity of metal/soft-donor complexes. **C. Phipps**, E. Hanna, A. Dickey, J.L. Brown-McDonald

CHED 1063. Catalytic activity of M-NHC complexes in polar organic and aqueous solvents. **M.B. Sebold**, R.J. Swails

CHED 1064. Extinction coefficient of germanium nanoparticles. **J.B. Lundervold**, K.A. Newton, S. Kauzlarich

CHED 1065. Suzuki and Heck coupling catalyzed by a Pd-NHC/pyridinium complex. **A. Conner**, R.J. Swails

CHED 1066. New trends in core size effect for oxygen reduction by quantized gold nanomolecules. **L. Sumner**, A. Antonysamy, S. Chakraborty, N. Sakthivel, K. Artyushkova, H. Schrock

CHED 1067. Synthesis of chiral sulfoxide ligands containing the 1-(4-methylnaphthyl)sulfinyl group. **C.N. Miller**, T.J. Brunker

CHED 1068. Synthesis and relaxivity of target-specific MRI contrast agents. **C. Clement**, J.E. Bradshaw

CHED 1069. Catalytic activity and nucleophilicity of a hydrolytic metalloenzyme mimic. **L. Carroll**, G. Tegenkamp, S. Peyer, A. Lajmi

CHED 1070. Examining novel adamantyl bearing Pd-PEPPSI complexes. **S. Hejnosz**, J.K. Vohs

CHED 1071. Cyclopentadienyl molybdenum N-Heterocyclic carbene complexes. **H.N. Hosack**, J.K. Vohs

CHED 1072. Creating nanostructured photoelectrochemical electrodes from iron oxide. **L.V. Morris**, J.E. Katz

CHED 1073. Reactions of transition metal oxides with fused NaOH-KOH eutectic mixture. D.A. Habboush, **O. Alkhudhari**, **K.M. Campos**, F.E. Divisconti

CHED 1074. Click compatible aminophenol ligands. **J.R. Farrell**, C. Adams, J. Connor Recio, S. Zaheer, C.J. Ziegler

CHED 1075. Preparation of titanium-chloride coordination complexes. **M. Shoukry**, B. Crabb, M.V. Bennett, L.G. Beauvais

CHED 1076. Effects of morphology on the luminescent properties of upconverting lanthanide doped phosphors. **C. Kinane**, J.T. Ippoliti

CHED 1077. Comparative study aimed at improving dye-sensitized solar cells. **H. Wakidi**, C.J. Timpson

CHED 1078. Constructing imidazole complexes of human serum albumin reconstituted with heme and testing for globin-like reactivities. **A. Alfonso Castro**, C.D. Kimrey, M.I. Galinato

CHED 1079. Synthesis of possible intermediates in the catalytic silylation of carbon hydrogen bonds. **N. Jocic**, R.M. Chin

CHED 1080. Synthesis and elucidation of a novel crystalline phase for a phosphonate-based biocompatible coordination polymer. **F.O. Fernandez**, G. Quiñones, I. Rodríguez, V. López-Mejías

CHED 1081. N-heterocyclic carbene catalysts for green chemistry hydrogenation. **K.B. Idrees**, E. Rajaseelan

CHED 1082. Synthesis, characterization and spectroscopic comparisons of tris(3-phenylpyrazolyl)borato zinc(II) and nickel(II) semiquinonate complexes derived from *in situ* oxidation of parent catecholate complexes. **C. Cox**, D. Isaacs, M. Bezpalko, N.A. Piro, W.S. Kassel, M.T. Kieber-Emmons, W.G. Dougherty

CHED 1083. Factors affecting absorbance readings of potassium permanganate. **D. Abaryan**, **S. Suh**, **K. Robles**, M. Mills, J. Bonilla, A. Manjikian, T.A. Boan

CHED 1084. Experimental and theoretical study of hydrogen production from an iridium hydride complex and empirically-based procedures for air-free chemistry. **E.D. Douma**, Z. Mathe, J.B. Tsang, M.A. Bowring

CHED 1085. Iridium hydride complexes for hydrogen production: Synthesis and mechanistic study. **J.B. Tsang**, Z. Mathe, E.D. Douma, M.A. Bowring

CHED 1086. Synthesis of organometallic vanadium complexes as antibiotic analogues. **N. Ciolkowski**, J.A. Dabrowski

CHED 1087. Synthesis and characterization of a model multi-copper oxidase. B.J. Johnson, **J. Gavin**

CHED 1088. Modifications to nickel diimine catalysts for polyethylene formation. **C. McCormick**, J.K. Vohs

CHED 1089. Dehydrogenative coupling of dimethylamine borane and chloroform. **B. Haslop**, G.M. Edvenson

CHED 1090. Complexation, extraction, and sensing of Hg(II) by thioamide ligands and analogs. **M.T. Fortunato**, I. Lehman-Andino, T. Jonah, O. Fernandez, K. Kavallieratos

CHED 1091. Mechanochemical synthesis of platinum compounds. **C. Taylor**, **J. Naidugari**, K. Williams

CHED 1092. Withdrawn

CHED 1093. Leaving ligand effects on solubility and reactivity of monofunctional platinum compounds. **H.L. Hruska**, K. Williams

CHED 1094. Synthesis and characterization of novel lanthanides with a macrocyclic ligand. **M. Gioia**, B.L. Westcott

CHED 1095. Synthesis and NMR characterization of acetyl-pyrazine methyl thiosemicarbazone and acetyl-pyrazine ethyl-thiosemicarbazone ligands: Formation of their Pd(II) and Pt(II) complexes. **K. Lawson**, D. Gardner, S.G. Bowman, X. Jiang, E.C. Lisic

CHED 1096. Synthesis and decarboxylation of tris(thione) copper carboxylate complexes. **J. Steets**, A.P. Honeycutt, J.M. Hoover

CHED 1097. Synthesis and characterization of pyruvic aldehyde-1-oxime thiosemicarbazones and their complex formation with Cu(II). **S.B. Crum**, S.G. Bowman, X. Jiang, E.C. Lisic

CHED 1098. Synthesis and characterization of new Anderson-Evans polyoxotungstate with iron(III) in its central cavity. **B. McKenna**, S. Nellutla

CHED 1099. Rhenium (I) tricarbonyls and their applications in anion sensing and CO_2 reduction. **D. Saugar**, M.O. Odago

CHED 1100. Halide and ligand effects on the fluorescence of thermochromic metal complexes. **I.V. Siepmann**, I. Wilt, A. Bowman

CHED 1101. Spectroscopic study of lanthanide complexation by tripodal tris-(pyrazolyl) ligands. **G.A. Flores**, T. Jonah, K. Kavallieratos

CHED 1102. Synthesis and NMR characterization of new AMOPY-TSC ligands and their Pd(II) complexes. **K.R. Lyons**, J.K. Allen, E.C. Lisic

CHED 1103. Catalytic synthesis of substituted benzimidazoles using metal phthalocyanines, pyridinoporphyrazines, and pyrazinoporphyrazines. **C. Genovese**, P.D. Voegel

CHED 1104. Sulfide oxidation for the removal of refractory sulfides from model oils via oxidative desulfurization with various polyoxometalates. **V. Anderson**, D. Thompson

CHED 1105. Synthesis of new redox mediators for dye sensitized solar cells. **J. Fitzgerald**, E.T. Papish, J.H. Delcamp, R.R. Rodrigues, O. Kuykendall, S. McKee

CHED 1106. Behavior of gold nanoparticles in aqueous environments. **S. Sobolewska**, J. Delph, H.S. Barcena, D. Berhanu

CHED 1107. Synthesis of pyruvaldehyde thiosemicarbazone (PTSM) metal complexes and their characterization by NMR. **A.C. Koch**, E.C. Lisic

CHED 1108. Synthesis, characterization, and electrochemical investigation of d^8-metal hydroxamate complexes. **A. Nikolai**, A. Warhausen

CHED 1109. Field XRF monitoring of heavy metal Pb^{2+}, Cd^{2+} and Zn^{2+} immobilization by fragmented and powdered shell beds from contaminated waters. **K. Kardas**, D. Rackie, S.K. O'Shea

CHED 1110. Characterization of alkanethiolate self-assembled monolayers on zinc selenide thin films. **S.K. O'Boyle**, A.R. Noble, N. Hellgren

CHED 1111. Revisiting zirconocene complexes for use as molecular photosensitizers. **M.E. Nally**, Y. Zhang, C. Milsmann

CHED 1112. Synthesis of nitrosolated metal dithiolates and bis-phosphine ligands as bridges in quadruply bonded dimolybdenum complexes. **R. Hodges**, C. Pectol, M.Y. Darensbourg

CHED 1113. Viability of inorganic synthesis methods for producing CdSe, CdS and ZnS quantum dots. **K. Beck**, T. Vinton, S. Lampa-Pastirk

CHED 1114. Validating the presence and exploring the role of a silver hydroxide intermediate in the production of silver nanoparticles. **D.A. Maldonado**, A. Loya, K.A. Beran, M.O. Montes

CHED 1115. Tetranuclear neutral titanium(IV)-based assembly from zigzag-shaped oligophenylene generated via a multicomponent self-assembly approach. **E. Day**, P. Mobian

CHED 1116. Using thermogravimetric analysis and X-ray data to determine how water is bonded in seven coordinate complexes. **S. Thibado**, J.H. Davis

CHED 1117. Direct growth of graphene on cobalt(II) oxide. **J. Castillo**, O.B. Olanipekun, C. Ladewig, J. Kelber

CHED 1118. The effect of chemical environment on the stability of metal-organic frameworks (MOFs). **D. Katic**, A. Spore

CHED 1119. Sequestraion of CO_2 by gamma cyclodextrin metal-organic frameworks. **M.F. Drew**, B.C. Manor, E. Maslowski

CHED 1120. Investigation of mesoporous silica for urea adsorption. **L. Veenstra**, B.J. Winters, K.E. Rohly

CHED 1121. Quantifying the thermodynamics of the surface modification of oleate-capped CdSe quantum dots with dodecylphosphonic acid via isothermal itration calorimetry. **Z. Di Giusto**, J.D. Keene

CHED 1122. H_2O_2 adducts of phosphine oxides: Safe, solid, stoichiometric, and soluble new oxidizing agents. **K.J. Angle**, F. Eberle, J. Bluemel

CHED 1123. Utilizing luminescence of europium(III) with chlortetracycline complexes as bioprobes. **T.A. Cabreros**, A.J. Riives, G. Muller

CHED 1124. Synthesis of new glyoxime-based electrocatalysts for small-molecule activation. **D. King**, A. Kumar, V. Day, J.D. Blakemore

CHED 1125. Synthesis and characterization of a novel copper (II) complex coordinated to a thiosemicarbazone ligand. **M. Rowand**, W.A. Weigand

CHED 1126. Synthesis and characterization of a copper (II) ethylene amine complex by an improved reaction methodology. **T. Adams**, W.A. Weigand

CHED 1127. Synthesis and characterization of new thiadiazole sulfonamide ligands reacted with copper (II) salts. **R. Peraino**, W.A. Weigand

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CHED 1128. Aqueous preparation of metal-organic frameworks for biomedical applications. **E.A. Morley**, **M. Mangun**, **J.W. Jamboretz**, **K.S. Malloy**, **N.D. Allen**, J.J. Pak

CHED 1129. Synthesis and characterization of copper(II) complexes supported by pyridylamide ligands. **J. Schneider**, L. Yang

CHED 1130. Synthesis and characterization of novel fluoro-bridged copper(II) complexes. **B. Johnson**, L. Yang

CHED 1131. Synthesis and structure of metallacrowns with varying alkali metal substitutions. **A. Kauffman**, C.M. Zaleski

CHED 1132. Synthesis and single-molecule magnet properties of metallacrowns with various bridging carboxylate ligands. **S. Nagy**, C.M. Zaleski

CHED 1133. Nickel-nickel dimers structurally reminiscent of common nickel scorpionates. **T.J. Clements**, P. Desrochers, N. Gerasimchuk

CHED 1134. Synthetic strategies for new thiocarboxylate-based metal-organic frameworks and their properties. **J.W. Jamboretz**, **K.S. Malloy**, **E.A. Morley**, **N.D. Allen**, **M. Mangun**, J.J. Pak

CHED 1135. Efficient preparation of R-scorpionate from R-boronic acids and microwave heating. **S. Margis**, P. Desrochers

CHED 1136. Modification of WSe_2 nanoplates created by screw dislocations. **J. Foster**, M. Shearer, S. Jin

CHED 1137. Effect of buffering agents on NP agglomeration in cement specimens during electrokinetic treatment. **A. Brown**, S.E. Eklund

CHED 1138. Surface modification of indium tin oxide substrates for depositing aqueous cobalt phosphate thin films. **A.T. Winegar**, R. Carter, C. Heideman

CHED 1139. Toward a low-valent, poly-electrochromic nanocomplex with up to 20-electron redox capacity. **D.A. Maldonado**, J.C. Applegate, M.V. Barybin

CHED 1140. Investigation of the antimicrobial mechanism of zinc oxide particles through morphological testing. **C. Beckley**, K. Casanova, A. Schnoebelen, B. Torrance, W.L. Cody, E. Steinmiller

CHED 1141. Synthesis and magnetic properties of cobalt(II)-pyrazine metal-organic frameworks. **D.V. Kravchuk**, J. Prybil, M.M. Kuntz, J.R. Parks, A. Ellern, P.M. Shand, C.L. Weeks

CHED 1142. Metal-organic framework polymer composite nanofibers for catalytic degradation of chemical warfare agent simulants. **D. Cooke**, D. Dwyer, W.E. Bernier, W.E. Jones

CHED 1143. Synthesis of 2-pyridinecarbaldehyde N-oxide. **K. Goerl**, P. Baran

CHED 1144. Synthesis of variable sized silver for the binding and delivery of drug derivatives. **A.N. Eubanks**, P.J. Rosado

CHED 1145. Preparation of in-situ regolith-based geopolymers for Martian structures. **R. Cooper**, S.E. Eklund

CHED 1146. Development of a repeatable solid state synthesis for educational labs. **K.L. Tracey**, B.J. Bellott

CHED 1147. Sol-gel synthesis and characterization of methylammonium perovskite compounds. **A.M. DiBernardo**, J.L. Hunting

CHED 1148. Synthesis and characterization of ruthenium and manganese CORM complexes with thiosemicarbazone ligands. **H. Daniels**, F.A. Beckford

CHED 1149. Development of new dithiazolyl and dipyrazolyl substituted formamidinate ligands for the stabilization of bimetallic and tetrametallic complexes. **S. Margaletta**, **S. Riley**, S.C. Haefner

CHED 1150. Interaction between chromate(VI) that has been reduced to chromium(III) and DNA. **S. Sinclair**, S. Brown, J.B. Vincent

CHED 1151. New β-hydroxy-acid ligands and their Al^{3+}, Fe^{3+}, and Ga^{3+}complexes. **W.H. Fitschen**, C.M. Davis

CHED 1152. Substituent and solvent effects on the magnetic properties of iron-based spin crossover complexes bearing hydrogen bonding groups. **M. Demmings**, A.M. Rabon, J.L. Payton, M.C. Young

CHED 1153. Reduction of KP1019/KP1339 using glutathione. **A. Rebic**, L.K. Stultz

CHED 1154. Synthesis, structure and reactivity of Ni(II) complexes with tridentate monoanionic ligands. **S. Lozowski**, M.J. Prushan

CHED 1155. Doping of $YIn_{1-x}Mn_xO_3$ with Cu, Gd, Sn, and Mo to form new inorganic pigments. **C.H. Levitt**, J.L. Hunting

CHED 1156. Investigating the chemistry of hexanuclear ruthenium cages and their trinuclear building blocks. **M. Niece**, F.A. Beckford

CHED 1157. Synthesis of $Ru(bpy)_3^{2+}$-rubredoxin-cobaloxime photocatalytic hydrogen evolution system. **A.M. Brown**, S.R. Soltau

CHED 1158. Synthesis of mono- and bi-metallic complexes of an β-diimine/dithiolene ligand. **G. Peng**, W.B. Heuer

CHED 1159. X-ray crystal structures of metal thiolates. C.D. Bryan, D.G. McGuire, **C. Iluno**, **J. Tidwell**

CHED 1160. Treating breast cancer with light: The creation of a photodynamic therapy agent. **V.F. Lackey**, J.E. Bradshaw

CHED 1161. Investigation of aluminum clusters. **M. Cole**, J.L. Bjorklund, T. Forbes, S.E. Mason

CHED 1162. Utilizing a simple molybdate catalyst, $[\{MoO(O_2)_2\}_2(\mu\text{-}O)]^{2-}$], for the β-oxygenation of ethers. **D. Schreurs**, D. Thompson

CHED 1163. Investigation of composite materials of chitosan and metal-organic materials in the inhibition of aggressive bacterial films. **J.C. Sessums**, **C.V. Gauthier**

CHED 1164. Oxygenation of organic sulfides with $[\{MoO(O_2)_2\}_2(\mu\text{-}O)]^{2-}$ grafted onto amine functionalized silica support. **K. Deheck**, D. Thompson

CHED 1165. Synthesis and characterization of new lithium calcium transition metal quaternary nitrides. **K. Gilbert-Bass**, J.L. Hunting

CHED 1166. Photocatalytic degradation of aqueous cyanide using compound parabolic reflector arrays. **E.R. Bishop**, J.M. Van Riper, J.E. Boyd

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Medicinal Chemistry

Cosponsored by MEDI and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 1167. Design and synthesis of a halogenated dibenzoxazepine library to probe antibiotic adjuvant activity in MRSA. **N. Cutrona**, K. Gillard, M.S. Blackledge

CHED 1168. Effects of low-frequency deep brain stimulation in the reinstatement of morphine place preference. **G. Sánchez-Navarro**, M.E. Lloret-Torres, F.J. Martínez-Rivera, J.L. Barreto-Estrada

CHED 1169. Role of lipid droplets in metastasis and drug resistance. **A.E. Hernandez**, S.C. Purdy, M. Wendt

CHED 1170. Isoform-selective docking with HADDOCK: Assessing the effects of protein conformation and score reliability using PI3Kβ. **E. Elder**, J. Grinstead

CHED 1171. Optimization of scale-up synthesis of anti-cancer ceramide Analog 315. **T. Hill**, T. Jackson, C. Do, S. Booker, M. Foroozesh, N. Goyal, J. Liu

CHED 1172. Synthesis of modified ZorO analogues for probing biological function. **H. Holst**, C. Gibson, B. Kennedy, S.R. Campagna

CHED 1173. Proton spin-lattice relaxation of pharmaceutical polymorphs by high resolution solid-state NMR. **B.E. Lininger**, J.M. Spehar, R. Quinones, R. Iuliucci

CHED 1174. Use of methyl scanning techniques in the development of novel ligands binding to the liver X receptor. **T. Nguyen**, **S. Kauloorkar**, **M. Woodruf**, K. Riley

CHED 1175. Synthesis of AAC(6')-Ib inhibitors to combat bacterial resistance to aminoglycosides. **L. Mellett**, **M. Pelkey**, M. Simes, Z. Cole, K. Jansen Labby

CHED 1176. Synthesis of novel ligands for platinum drugs. **W. Jones**, **A.E. Fraeyman**, R.A. Banner, A.J. Carnathan, D.A. Lee, K. Providokhina, C.S. Chow, K.J. Friedrich

CHED 1177. Met-enkephalin: A pharmaceutical treatment for the symptoms of post-traumatic stress disorder. **K. Striker**, J. Thomson, R. Kroeker Sachs, N. Balten, J. Davis, E. Harkens, K. Jacunski, H. Rohland

CHED 1178. Asymmetric synthesis of fluorine substituated β-lactams as leads to advanced anti-bacterial organics. **B. Gamelin**, J.C. Easdon

CHED 1179. Analysis of a myelin sheath model membrane system with the addition of ginkgo biloba flavanols. **R.A. Book**, A. Sostarecz

CHED 1180. Design, synthesis, and evaluation of 1,2-dihydroquinazolin-2-ones against *Trypanosoma brucei*. **M.E. Walden**, T. Pham, C.R. Butler, H. Zecca, E. Krakoff, B. Kopec, O. Ichire, C. Mackenzie, M. Pitot, M. Navarro, G. Ceballos-Pérez, R. Diaz-Gonzalez, A.B. Dounay

CHED 1181. Specific, homologous peptides designed to mark Aβ42 oligomers for microglial clearance. **M. Burlette**, R. Cooper, J. Rodrigues, M.A. DeCoster, S. Poh

CHED 1182. Inhibition of *Botrytis cinerea* with Terpinen-4-ol. **J. Walsh**, D. Little, K. Anderson

CHED 1183. *Bromelia pinguin* aerial root extract induces HeLa cell apoptosis: MTT assay-supported. **S. Luna**, S. Deprele, L. Nogaj

CHED 1184. mTOR inhibition increases lifespan in Li-Fraumeni Syndrome fibroblasts by positively influencing the DNA damage response. **L. Levy**, L. Amar, R. Kafri, D. Malkin

CHED 1185. Natural remedies and cancer in women: A peruvian communities survey study. **R. Moran**, **K. Guzman**, **D. Morales**, **S. Luna**, **S. Deprele**, **L. Nogaj**, **L. Roberts**

CHED 1186. Styrylquinoline: A scaffold for the next generation of antimalarials. **J. Kreisel**, B. Roberts, Y. Zheng, D. Chakrabarti, Y. Yuan

CHED 1187. Effects of maternal care and energetics on neural activation patterns in the African cichlid fish, *Astatotilapia burtoni*. **C. Forester**, K. Field, K. Maruska

CHED 1188. *Invivo* studies on non-toxic polysaccharide based delivery systems for chemotherapy treatment. R. Srinivasan, J. Speshock, D. Edwards, **J.D. Murphy**, L. Hernandes, J. Orona, A. Palumbo, **M. Cardenas**, **D. Bocanegro**

CHED 1189. Progress toward a photo-switchable kinase inhibitor. B. Swartz, **P. Sheperd**, C. Streu

CHED 1190. Synthesis of a photoisomerizing azologue to inhibit ALK5. **L.E. Kelsey**, T. Hall, C. Streu

CHED 1191. Utilizing light sensitive ruthenium complexes to target cancer. **A.R. Hairston**, S. Altman, J. Gray, F. Qu, J. Park, Y. Kim, E.T. Papish

CHED 1192. In vitro studies on non-toxic polysaccharide based delivery systems for anti-cancer drugs. R. Srinivasan, J.D. Murphy, **L.G. Hernandez**, J. Speshock, D. Edwards, J. Orona, **A. Palumbo**, M. Cardenas, D. Bocanegro

CHED 1193. Preparation of synthetic analogs of Modafinil. **A. Williams**, W.R.

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Winchester

CHED 1194. Synthetic strategies for novel fluorinated pyronins. **F. Boumelhem**, Z. Woydziak

CHED 1195. Recent progress on the synthesis of a methotraxate derivative to be used in ADEP therapy. M.J. Rouffet, **K. McFarland**

CHED 1196. Protonatable dipyrrinones: Synthesizing a library of fluorescent pH probes. **N. Benson**, Z. Woydziak

CHED 1197. Synthesis of aminopyonin analogs and their biological use. **A. Johnson**, J. Newby, A. Kibbe, Z. Woydziak

CHED 1198. Synthesis and biological testing of chalcone derivatives. **C.J. Leatherwood**, S. Greer, A.L. Thomas, G. Cuadra

CHED 1199. Synthesis and anti-proliferative activity of *N,N'*-bis-substituted triazolium salts with various substituents. **Z. Lin**, C. Cardenas, J. Bies, J.D. Gorden, J. Strickland, M. Frazier, J.M. Meyers, K.L. Shelton

CHED 1200. Extraction and fractionation of polyphenols from Peruvian teas and their effect on mammalian cell viability. **D. Morales**, R. Moran, S. Deprele, L. Nogaj

CHED 1201. Continued progress toward a novel synthetic pathway to Aspernigrin A. **D. Lemen**, Z. Cross, D. McDermond, A.M. Reeve

CHED 1202. Chemical extraction, biological evaluation, and stability analysis of coastal Maine *Saccharina latissima* extracts that exhibit antimicrobial potency against MRSA. A.M. Deveau, K.M. Burkholder, Z. Miller-Hope, **A.J. Cusson**

CHED 1203. Synthesis of unique lubricants made of exotic butters infused with indigenous oils to promote inhibition of bacteria and protection against UV radiation. **M. Lopata**, K. Melkonian, J.I. Rizzo

CHED 1204. Novel antimicrobial surfaces derived from beeswax infused with exotic oils. **L.Z. Shapiro**, K. Melkonian, J.I. Rizzo

CHED 1205. Towards a new immobilization motif of cell adhesion peptides on titanium. **E.R. Leung**, A.M. Blystone, E.S. Gawalt

CHED 1206. Localized drug delivery of aspirin to stent sites via self-assembled monolayers. **A. Miskalis**, T.M. Lovelace, A. Blystone, E.S. Gawalt

CHED 1207. Increase colistin susceptibility in antibiotic resistant *Pseudomonas aeruginosa*. **M. Tran**, L.C. Miller Conrad

CHED 1208. Analysis of the apoptotic behavior of neutrophils in antipsychotic-induced neutropenia. **C. Swain**, P. Cavnar

CHED 1209. What Influence does parabens and paraben derivatives have on T cell immunity? **H. Kintz**, A.A. Yeagley, A. Barber

CHED 1210. Investigating the structure activity relationship of the ester moiety in parabens through the analysis of bioisosteres. **K. Jones**, **A.A. Yeagley**

CHED 1211. Investigating the synergy between paraben derivatives and the antibiotics penicillin and erythromycin. **K. Jeffeson**, A.A. Yeagley

CHED 1212. Repurposing the FDA-approved raloxifene to potentiate gemcitabine cytotoxicity in pancreatic cancer. **J. Trinh**, A. Badejo, Q. Love, H. True, D. Rao, A. Malhotra

CHED 1213. Development of selective kappa opioid receptor ligands. **H.W. Karstens**, N. Ramirez, D. Toth, B.A. Provencher

CHED 1214. Disruption of bacterial communication by targeting LuxI-type synthase CviI. **T. Nguyen**, A. Balistreri, M. Aguilar, A. Chavez, M. Gomes, A. Jiu, L.C. Miller Conrad

CHED 1215. Synthesis and biological evaluation of new ceramide analogs containing a flavone moiety. **C. Do**, M. Hill-Odom, T. Ponnapakkam, N. Goyal, M. Foroozesh

CHED 1216. Antibiotics from actinomycete bacteria with activity against *E. coli*. **J. Chung**, A. Hoffman

CHED 1217. Synthesis of an amine containing antibacterial. **A.N. Roux**, J.T. Ippoliti

CHED 1218. Synthesis of a novel oxazolidinone antimicrobial agent. **T.J. Ogorek**, J.T. Ippoliti

CHED 1219. Synthesis and characterization of novel diphenyl urea antibiotics. **P.C. Dietz**, K.M. Nauta, M.E. Hart

CHED 1220. Will a change in the leaving group affect the rate and/or the mechanism of ROCOX solvolytic reactions? **J.J. Wirick**, M.J. D'Souza

CHED 1221. Introduction of a liquid chromatograph-mass spectrometer to the discovery of antimycobacterial compounds from marine bacteria. **J. Dang**, J.A. Trischman

CHED 1222. Synthesis and evaluation of heterocyclic biaryls as aggregation inhibitors for Alzheimer's amyloid-beta peptide. **B. Hernandez**, M.G. Murray, B.L. Crenshaw, A.V. Vinson, M.J. Hurtt, R.K. Lammi, J.M. Hanna

CHED 1223. Evaluation of organic solvents and thiazolidine-2-thiones for bacterial growth and biofilm inhibition. **S.C. Wallin**, T.J. Eckroat

CHED 1224. Synthesis of multicolor fluorescent ligands for nicotinic acetylcholine receptors. **A.N. Davis**, R.W. Fitch

CHED 1225. Use of cytosine-based tautomerically ambiguous nucleosides for induction of viral mutagenesis. **C.M. Clem**, V.K. Dunlap

CHED 1226. DNA binding studies of a copper 12-MC-4 metallacrown. **E. Manickas**, C.M. Zaleski, **A. Hurley Predecki**

CHED 1227. Biological studies of ceramide analogs towards the treatment of breast cancer. **T. Saulsberry**, T. Jackson, T. Hill, M. Hill-Odom, T. Ponnapakkam, N. Goyal, J. Liu, M. Foroozesh

CHED 1228. DNA binding and intercalation studies of aryl sulfoxides. **M. Doleschal**, A. Hurley Predecki

CHED 1229. Synthesis of a novel oxazolidinone antibacterial agent containing an alcohol functional group. **B. Kraemer**, J.T. Ippoliti

CHED 1230. Synthesis and biochemical evaluation of piperine analogs for acetylcholinesterase inhibition. **M.N. Horn**, **T. Soto Torres**, T.J. Eckroat

CHED 1231. Synthesis of novel acyl hydrazones as inhibitors for fungal GlcCer synthesis. **J.E. Zambito**, K. Haranahalli, Y. Sun, C. Lazzarini, M. Del Poeta, I. Ojima

CHED 1232. Antimicrobial studies of monolignol compounds. **A.N. Winters**, L.J. Moore

CHED 1233. Promising anti-pancreatic cancer compound: Investigations into combination therapies and stability of DCM-MJ-I-21 in vehicle. **E. Wang**, E. Kusaka, A. Webb, D. Carrico-Moniz

CHED 1234. Design and syntheses of new dibenzofuranol ether derivatives as potential cytochrome P450 inhibitors. **K.M. Williams**, M. Hill-Odom, N. Goyal, M. Foroozesh

CHED 1235. Synthesis of guanidino derivatives of aryl-substituted polyamines as inhibitors of *Trypanosoma cruzi* trypanothione reductase. **T. Utz**, M. Rizzo, **M. Smardz**, M.C. O'Sullivan

CHED 1236. *N*-Isopropyl derivatives of aryl-substituted polyamines: Synthesis and inhibition of trypanothione reductase. **M. Smardz**, M. Rizzo, **T. Utz**, I. Kozik, M.C. O'Sullivan

CHED 1237. Efficacy of specific polyphenolic compounds epigallocatechin gallate and gallic acid as antibacterial eluents in a macroscale polymeric drug delivery system for surgical sutures. **N. Borkowski**, D. Fish

CHED 1238. Synthesis of compound 10221 for peroxisome proliferator-activated receptor interactions. **T. Clark**, T. Hughes

CHED 1239. Advancements in magnetic resonance imaging: Synthesis of a bromo-functionalized macrocyclic pyrinophane ligand. **E.R. Dobias**, C. Galaup

CHED 1240. The synthesis of a novel oxazolidinone anitbacterial derived from dopamine. **T.J. Higgins**, J.T. Ippoliti

CHED 1241. Computational modeling of a new series of somatostatin subtype 4 receptor agonists. **O. Slater**, A. Hospital, K. Sandoval, M. Kontoyianni

CHED 1242. Kinetic characterization of human low molecular weight protein tyrosine phosphatase wild type isoforms A and B. **S.L. Tinucci**, H.V. Jakubowski, E.J. McIntee

CHED 1243. Exploring early connections to the modern opioid crisis. **B.A. Steele**, C. Street

CHED 1244. Withdrawn

CHED 1245. Antimicrobial activity of penicillin in combination with potential beta-lactamase inhibitors. **S. Greer**, A.L. Thomas

CHED 1246. Synthesis and biological evaluation of a new series of sulphonamide-containing ceramide analogs. **S. Booker**, N. Goyal, M. Foroozesh

CHED 1247. Exploration of medicinal compounds in Peruvian spices and their effect on cervical and breast cancer. **P. Perez**, R. Solomon

CHED 1248. Phenotypically distinct cubset of eosinophils is recovered with intestinal Intraepithelial leukocytes. **Y. Huang**, D. Anketell, J.J. Xenakis, K. Smith, C.L. Olbrich, E.W. Cornwell, E.D. Howard, L.A. Spencer

CHED 1249. Synthesis and investigation of a novel antimicrobial surface utilizing agar. **A.J. Sostre**, K. Melkonian, J.I. Rizzo

CHED 1250. Exploring evolutionary medicine through 19th century medical collections: Applications in archival studies. **T. Sturgill**, C. Street

CHED 1251. Monoacylglycerol lipase inhibition blocks gastric hemorrhages induced by the cyclooxygenase inhibitor diclofenac sodium. **H. Aliff**, M. Eckard, E. Silvestri, K. Trexler, M. Crowe, S. Kinsey

CHED 1252. Human serum albumin nanoparticles for drug delivery and release: Developing alternative treatments. **M. Hibino**, M.A. Tarr

CHED 1253. Fragment-based synthesis and biological evaluation of antimicrobial peptide derivatives. **A. Corkovic**, E.K. Leggans

CHED 1254. Development of novel chemotherapeutic agents via the Maillard reaction. **N. Hmeluk**, R. Sheaff

CHED 1255. Synthesis and biological evaluation of xenortide derivatives. **V. Cheslack**, E.K. Leggans

CHED 1256. Oleate rescue of lipotoxicity. **B. Berg**, A.K. Stoeckman

CHED 1257. Biological evaluation of antimicrobial peptide analogues. **Z. Spahr**, M. Pietrusiak, E.K. Leggans

CHED 1258. Cellular mechanisms of lipotoxicity. **E. Inwards**, A.K. Stoeckman

CHED 1259. Synthesis of 2(2-trifluoromethylsulfonamidephenyl) benzimidazole derivatives as IspF inhibitors for the development of novel antibiotics. **D. Harper**, M.J. Rouffet

CHED 1260. Effects of ultraviolet A and ultraviolet B radiation on melanoma cells. **D. Carlsen**, K.S. George Parsons

CHED 1261. Recent progress on the development of anthrax lethal factor inhibitors. **S. Veenbaas**, M.J. Rouffet

CHED 1262. Syntheses of 4-bocpiperidone chalcones and their potential as anticancer agents. **T.A. Pereles-De-León**, C. Vélez-Gerena, B. Zayas, M.J. Donate, M.M. Sánchez, M.

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Martínez-Ferrer, D.J. Sanabria-Rios

CHED 1263. Influence of chronic restraint stress during adolescence on brain-derived neurotrophic factor (BDNF) hippocampal expression in adult male and female rats. **M. Bhardwaj**, K. Krolick, E. Gulla, S. Marshall, H. Shi

CHED 1264. Preparation of docetaxel (Dxtl)-encapsulated poly (lactic-co-glycolic acid) (PLGA) nanoparticles (NPs) and their potential as anticancer agent against highly metastatic prostate cancer cells. **G. García-Robles**, **K. González-González**, E. Nicolau, M.J. Donate, M.M. Sánchez, M. Martínez-Ferrer, D.J. Sanabria-Rios

CHED 1265. Isolation, purification, and characterization of the zwitterionic polysaccharides, PS-A1 and Sp1. **G.T. Hymel**, P.R. Andreana

CHED 1266. Optimal scaffold flexibility permits backbone polarity exclusion during passive membrane permeation in bRo5 peptide macrocycles. **M. Handford**, M. Naylor, A. Ly, S. Lokey

CHED 1267. HIV-1 envelope glycoprotein trimeric immunogens derived from donor 45 envelope sequences form highly stable and native-like trimers. **J. Santiago Echevarria**, J. Guenaga, B. Carrate, R. Wyatt

CHED 1268. Synthesis of an esterified calcein through a Friedel-Crafts-like reaction, by first synthesizing a modified resorcinol through a Mannich reaction, in order to make a membrane impermeable clickable fluorescent probe. **B. Roman**, M. Fiore, G. Leveau, D. Fayolle, P. Strazewski

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Nanochemistry

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 1269. Efficient dual-site carbon monoxide electro-catalysts via interfacial nano-engineering. **D. Falkner**, Z. Huang, Z. Wang, Z. Liu

CHED 1270. Withdrawn

CHED 1271. Electrochemical properties of tin-coated vertically aligned carbon nanofiber array anode for Li-ion storage. **K.J. Jones**, G.P. Pandey, L. Meda

CHED 1272. Ionic conducting property of poly(propylene carbonate) interpenetrating cross-linked poly(ethylene glycol) network. L. Meda, Y. Yang, **J. Williams**

CHED 1273. Nickel-carbon composits as electrodes for the methanol oxidation reaction. **A. Reid**, K.M. Metz

CHED 1274. Controlled patterning of carbon nanotube growth utilizing polymer thin films. **I. Frenkel**, J.N. Albert, N. Pesika

CHED 1275. Print-welding functional biopolymer composites. **S. Park**, R. Chung, D.P. Durkin, L.M. Haverhals, H. De Long, P.C. Trulove

CHED 1276. Protein corona formation: Investigating the effects of cell culture growth media on nanoparticle size, stability, and net charge. **Y.I. Avila**, D.P. Simmons, M.A. Omary

CHED 1277. Effect of silver-based antibiotic infused nanofibers on bacterial growth and drug delivery. **A. White**, **J. Jones**, K. LaiHing

CHED 1278. Alloy Au/Ag nanoparticles introduced to yeast cells *in vivo*. **F. Falcon Ontiveros**

CHED 1279. Novel characterization of silver nanoparticles utilizing a laser system. **N. Hernandez**, K.A. Beran

CHED 1280. Scattered photon intensity as a tool to calibrate the size of Au and TiO_2 nanoparticles. **L. Ramirez**, K.A. Beran

CHED 1281. Colorimetric detection of DNA via catalytic release of polymer bead-immobilized gold nanoparticles. **C. Bonner**, D. Moyer, D. Lysne, J. Sigurdson, A. Nguyen, E.D. Graugnard, J. Lee

CHED 1282. Synergestic effects of organic nanofibers, honey and antibiotics for wound dressings. **C. Stewart**, S. Parkins, K. LaiHing

CHED 1283. Incorporation of silver-based antibiotic in maltose nanofibers for drug enhancement. **A. Saunders**, N. Fleary, K. LaiHing

CHED 1284. Aqueous phase transfer of $CuInS_2$/ZnS nanocrystals for toxicity studies. **C. Peterson**, S. Hughes
CHED 1285. Using layer-by-layer deposition to "trap" polyelectrolytes on gold nanoparticles. **A.V. Murray**, K. Andresen, L.B. Thompson

CHED 1286. Spectroscopic quantification of fluoxetine-loaded polyacrylamide linked to the surface of gold nanoparticles. **R.J. Gawel**, P.P. Fong, L.B. Thompson

CHED 1287. New solid polymer substrate containing gold nanoparticles. **B.A. Bober**, B. Negru

CHED 1288. Using pH to drive assembly of poly-l-lysine coated gold nanorods. **F.E. McFeaters**, L.B. Thompson

CHED 1289. A facile synthesis of pectin-coated silica nanoparticles. **G. Elizondo**, **F. Elizondo**, E. Evans, B. Mellis, J. Hollingsworth

CHED 1290. Two step syntheses of NiFe-P nanosheets as electrode materials for supercapacitors. **Z. Johnson**, J. Luo, Z. Zheng, W. Zhou

CHED 1291. Stability of C_{60} fullerene solutions in vegetable oils. **L.D. Bienski**, R. Ortiz-Ayala, K.R. Warnke, C.A. Torres

CHED 1292. Investigation of a nanoscale surface area coverage by a self assembly of amyloidogenic peptides. **P. Shevlin**, K. Yokoyama, K. Brown

CHED 1293. Repurposing the anticancer drug cisplatin for a post-antibiotic era. **M. Foronda**, E. Michael

CHED 1294. Analyzing synergistic interactions between silver nanoparticles and antibiotics: Implications for microbial growth. **E. Stuffle**, N. Sakyi Opoku, M. WaMaina, C. Stewart, E. Vanterpool, K. LaiHing

CHED 1295. Comparison of synthesis methods for Au nanoparticles. **F.P. Verdin**, M.G. Weir

CHED 1296. Repairing degenerately-doped nanocrystal films by gallium diffusion. **S.D. Mengel**, A.T. Fafarman

CHED 1297. Electrochemical and electrogenerated chemiluminescence study of organolead halide perovskite nanocrystals. **V. Arau**, Y. Wusimanjiang, S. Pan

CHED 1298. Homogeneous nucleation-driven formation of gold nanoprisms: A real time spectroscopic and microscopic investigation. **M. Kaur**, T. Liyanage, M. Agarwal, R. Sardar

CHED 1299. Fully solution processed semitransparent inorganic nanocrystal solar cells. **E. Donahue**, N. D'Antona, T. Townsend

CHED 1300. Probing the distance-dependence of surface-enhanced Raman Spectroscopy using nanocomposites composed of raman reference and probe conjugated copolymers grafted to gold nanoparticles. **S. Best**, E.G. Westbrook, P. Zhang

CHED 1301. Detection of testosterone through host-guest interactions of β-cyclodextrin functionalized silver nanoparticle. **A.A. Hill**, D. Buker, A. Deckert

CHED 1302. Porous metal-organic frameworks for hydrogen storage. Y. Liu, **P. Farias**

CHED 1303. Synthesis & characterization of cysteine derivatives for quantum dot growth. **S. Yang**, P.E. Lee

CHED 1304. Interaction of silver nanoparticles with cardiovascular drugs on *Daphnia magna*. **P. Garcia Gonzalez**, Y. Santos Vazquez, E. Ferrer Torres

CHED 1305. Synthesis of polymer/polyoxometalate multilayered gold nanoparticles. **C.N. Banson**, **B.T. Nhan**, S. Valcin, N.T. Flynn

CHED 1306. Thiol-ene photopolymerization of functionalized resorcinarene cavitand thiols. **S. Johnston**, S.D. Allmon, B. Ramjee

CHED 1307. Luminescent gold nanoparticles for sensing chromium (III) ions in physiological environment. **A. Lanzendorf**, C. Zhou

CHED 1308. Surface engineering of nanostructured electrodes and electrolytes for solid-state battery applications. **A.C. Mesnier**, D.C. Teeters

CHED 1309. Charcoal-based conductive paint. **A. Wyatt**, W.E. Schatzberg

CHED 1310. Nitric oxide-releasing materials for the remediation of microbial growth on cultural heritage items. **T.Y. Dilday**, R.A. Hunter

CHED 1311. Electrocatalytic detection of single Pd, Pt, and Rh nanoparticles at Au and Hg ultramicroelectrodes. **A.J. Capps**, S.N. Thorgaard

CHED 1312. Detection of sports doping drugs using noble metals nanoparticles. **A. Ruiz Ferrer**, M. Negron Garcia, E. Ferrer Torres

CHED 1313. Development of size-matched nanoparticles–silicon dioxide and gold for small organic compound detection. **L. Sanford**, E. Magennis, J.S. Kirk

CHED 1314. Synthesis of silica@gold core shell nanoparticles and their interaction with Capacetabine (an anti cancer drug). **F. Rodriguez Reyes**, J. Santiago Echevarria, E. Ferrer Torres

CHED 1315. Biomarker detection with different nanoparticles: A comparative analysis between plasmonic nanoparticles and quantum dots. **S. Szajek**, J.M. Wiester

CHED 1316. Using $CuFeS_2$ nanocrystals for solar-to-steam energy conversion. **A. Mapile**, V. Holmberg, B. Bishop, S. Lee

CHED 1317. Deposition and sintering techniques to strengthen silica nanoparticle crystals. **M. Koviekis**, S. Bingham, J.S. Kirk

CHED 1318. Synthesis and study of Ag, Au and Ag/Au nanoparticles for the detection of heavy metals and toxic agents in water samples. **C. Cabrera Lopez**, A.G. Colon Santiago, E. Ferrer Torres

CHED 1319. Synthesis of lipid-polymer hybrid nanoparticles: A drug delivery system. **J. Centore**, D. Fish

CHED 1320. Investigating protein adsorption on functionalized gold nanoparticles. **A.L. Code**, **M.T. Phan**, A. Uchitelle, A. Webb, N.T. Flynn

CHED 1321. Silicon monoxide nanoporous membranes for lithium ion battery anode. **N. Johnson**, J. Wu

CHED 1322. Fine-tuned nanoparticles synthesis for controlled pore size and condensation degree. **E. Hjelvik**, A. Noureddine, J. Agola, J. Croissant, C. Brinker

CHED 1323. Functionalization of gold nanoparticles with multiple stabilizing agents. **A. Uchitelle**, N. Al-Qadi, N.T. Flynn

CHED 1324. Size-dependent optical properties of cadmium selenide quantum dots. **C. Henderson**, M. Quackenbush, K. Schnitzenbaumer

CHED 1325. Synthesis and characterization of cadmium-free nanomaterials. **S. Hernandez**, K. Schnitzenbaumer

CHED 1326. Assessment of catalytic function of gold nanorod-bound TEMPO under NIR irradiation. **K. St. Clair**, K. Lavan, J.W. Stone

CHED 1327. Photothermal treatment of A-375 melanoma cells containing gallic acid capped gold nanoparticles. **T.J. Dominguez**, S. Huynh, E. Evans, A. Gorman, A. Tjandra, C. Flores, M. Steiger, B. Mellis

CHED 1328. Assessing the spontaneous nanorod linkages driven by the PEG on the GNR surface. **M. Braselton**, J.W. Stone

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CHED 1329. Evaluation of coated gold nanorods on zebrafish embryos. **J. Smith**, M. Braselton, V. Sittaramane, J.W. Stone

CHED 1330. Carbon nanotube and transition metal oxide composites via microwave synthesis. **M.D. Havlik**, J. Zemke

CHED 1331. Synthesis, characterizations, and potential applications of Au-Ir nanoparticles. **D.S. Fernandez**, H. Guo, S.M. Humphrey

CHED 1332. The identification of bacterial isolates from cationic nanoparticle solutions and their interactions with cationic gold nanoparticles. **J.E. Kuether**, R. Tapia Hernandez, V. Feng

CHED 1333. Using EC-STM to study the binding of amino acids to metal surfaces. **I. Baljak**, J.A. Phillips, L.K. Harville, E.V. Iski

CHED 1334. Self-assembly of PbS Nanocrystals in thin Films. **C. Cuthbert**, W.B. Heuer

CHED 1335. Electronic properties of porphyrin nanowires. **M.L. Buzbee**, M.B. Elinski, T. Reyes, J. Batteas

CHED 1336. Synthesis of Au nanorods with Pd4 peptide-capped Pd nanoparticles functionalization for Suzuki coupling reactions. **J. Wagner**, B. Briggs, M. Smith

CHED 1337. Removal of heavy metals from aqueous solutions by alginate-AgAu nanoparticles composite. **J.G. Noel Torres**, C.B. Pellicier Rodriguez, C.M. Osorio Cantillo

CHED 1338. Direct growth of iron oxides on stainless steel as anode for Li-ion batteries. **K. Strong**, Y. Yang, L. Meda

CHED 1339. Investigate the effects of DNA structures and their interactions with gold nanoparticle surfaces. **L. Pierce**, J.E. Smith

CHED 1340. Pseudocapacitive study of NiO nanomaterials for electrochemical energy storage. **A. Day**, J. Adkins, L. Meda

CHED 1341. Gold nanorod-protein composites as a potential novel therapy for alpha-1-antitrypsin deficiency. **M. Kilpatrick**, J.W. Stone

CHED 1342. Vapor synthesis of MnO nanoparticles embedded in a carbon matrix as high performance anode for lithium-ion batteries. **N.X. Tran**, L. Leban, Y. Yang, L. Meda

CHED 1343. Electrochemical studies of RuO_2 reactions with lithium ion. **A. Merrell**, J. Adkins, J. Williams, Y. Yang, L. Meda

CHED 1344. Bifunctional peptide for synthesis of Fe_3O_4 and Pd nanoparticles for recycling in Suzuki coupling. **S. Castillo**, B. Briggs

CHED 1345. Amorphous niobium oxide thin film as anode for high rate lithium ion battery. **K.A. Kimble**, N.X. Tran, A.A. Abiade, J.I. Adams, J. Adkins, L. Meda

CHED 1346. Studies of Lipon coated metal oxides in lithium ion battery conversion reaction. **E. Marin**, S. Desselle-Hirsch, J. Callaway, L. Meda

CHED 1347. EC-STM investigation of the thermal stability of silver halide thin films on Au(111). **L.K. Harville**, J.A. Phillips, I. Baljak, E.V. Iski

CHED 1348. Surface attachment of insulin upon nanodiamonds. **A. Arshi**, M. Su, B. Negru, H. Shi

CHED 1349. PVP-assisted synthesis of uniform carbon coated Li_2S/rGO for high-performance lithium-sulfur batteries. **J. Adkins**, G.P. Pandey, L. Meda

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Organic Chemistry

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N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 1350. Low band gap *p*-conjugated molecules featuring NβB coordination. **J.L. Lavoie**, C. Zhu, L. Fang

CHED 1351. Synthesis of polyaromatic hydrocarbons via mechanochemistry. **B. Theard**, J. Mack

CHED 1352. Preparation of novel ligands for the dynamic kinetic resolution of β-amino acids. **E. Allbritton**, **A. Bond**, **S. Crone**, **E. Hicks**, K. Kemp, **D. Tresp**, **D. Widick**, S. Hamburger, P.M. Wright, T.K. Ellis

CHED 1353. General mild method for cleavage of methoxymethyl ethers using bismuth trichoride. **A. Pacherille**, B. Tuga, I. Dos Reis, R. Sunasee

CHED 1354. Redox auxiliary mediated *Z*—>*E* switching of a stable *cis* azobenzene. **C. Meyers**, D. Warner, S.C. Blackstock

CHED 1355. Synthesis and photophysical properties of bindone derived heteroaryl dienes. **C. Roberts**, S. Helmy

CHED 1356. Solid-state studies of halogenated benzonitrile oxides and their dimers. **M. Stodolka**, W.H. Ojala

CHED 1357. Microwave assisted organic synthesis and purification of various N-phenyl succinimides derivatives. T.F. Guetzloff, **J.D. Simms**, M.B. Guetzloff, M.W. Fultz

CHED 1358. Molecular structure similarities vs. crystal structure similarities: *bis*(4-Chlorophenyl)furoxan vs. *bis*(4-methylphenyl)furoxan. **S. Whitcomb**, W.H. Ojala

CHED 1359. Microwave synthesis of various N-phenyl succinimide derivatives. T.F. Guetzloff, **M.B. Guetzloff**, M.W. Fultz

CHED 1360. Bisulfite extraction of aldehydes and reactive ketones: Extraction optimization and re-isolation of alpha chiral aldehydes without racemization. **M.H. Furigay**, **M.M. Boucher**, N.A. Mizgier, P.K. Quach, C. Brindle

CHED 1361. Microwave synthesis of N-phenyl succinimides and adaptation in organic chemistry laboratory. **T.F. Guetzloff**, M.W. Fultz, M.B. Guetzloff

CHED 1362. Isomorphism in heteropentacycles: Crystal structure of a 1,2,4-oxadiazole and comparison to its isosteric analogues. **M. Neuzil**, W.H. Ojala

CHED 1363. Fluoroamide-directed fluorination of unactivated C–H bonds. **J. Bingham**, B.J. Groendyke, S.P. Cook

CHED 1364. PEG-based increases to conformational and proteolytic stability of a β-sheet protein depends on PEGylation strategy and location. **N.A. Becar**, S.R. Draper, P.B. Lawrence, W.M. Billings, Q. Xiao, N.P. Brown, D.J. Matheson, J.L. Price

CHED 1365. Improved synthesis of a highly soluble calix[4]arene- capped azobenzene. **L. Scharlott**, A.A. Darling, P.A. Bonvallet

CHED 1366. Progess towards the synthesis of mono-and dibenzal quinoxaline-spanned heterocapsules. **M. Lopez**, J. Ruiz, L.M. Tunstad

CHED 1367. Comparing solvent effects between resorcin[4]arene homologs. **J. Woojuh**, **D. Moreno**, **G. Walker**, L.M. Tunstad

CHED 1368. Synthesis of a short-tethered calixarene-capped azobenzene. **J. Shea**, **C.A. Litts**, C.M. VanDenburgh, P.A. Bonvallet

CHED 1369. Diastereoselective synthesis of a single diastereomer dipeptide analog in the Ugi reaction via the use of chiral *N*-acylhydrazone auxiliaries. **X. Zhu**, A. Davies, M.T. Peterson, A. Baker

CHED 1370. Cobalt-catalyzed hydroboration of 1,3-(*E*)-dienes. **M. Mehta**, T. Rajanbabu

CHED 1371. Synthesis and analysis of pyrazoline derivatives as alcohol dehydrogenase inhibitors. **M.E. Hackey**, L.L. Rossi

CHED 1372. Exploration of the role of base in selective phosphorylations. **E. Sisko**, B.R. Sculimbrene

CHED 1373. Rapid synthesis of N-methyl-N-(2-nitrobenzyl)formamide. **S.E. Sundhagen**, L.I. Bobyleva, M.M. Bobylev

CHED 1374. Synthesis of azuliporphyrins from 2-methylazulene. **J.D. Moriones**, T.D. Lash

CHED 1375. Intermolecular-trapping of 1,3-dialkyl diaziridines with HDDA-derived benzynes. **R. Rupasinghe**, S. Arora, T.R. Hoye

CHED 1376. Synthesis of bidentate, unsymmetric N-heterocyclic carbene ligands for potential applications in cis-selective olefin metathesis. **A.C. Edwards**, L.P. Bryant, K.D. Leibfried, H.J. Schanz

CHED 1377. Development of the formation of nitrogen-nitrogen bonds as a tool for synthesis and drug development. **B. Davis**, A. Reeder, A. Wollenburg, M.R. Prinsell

CHED 1378. Molecular switching of bis(azobenzene)aniline. **T.F. Morgan**, K.S. Strickland, S.C. Blackstock

CHED 1379. Synthesis and characterization of 5,10,15,20-tetrakis(4-hydroxy-3-methoxy-5-nitrophenyl) porphyrin. **A. Adeyemo**

CHED 1380. Photo-Nazarov reactions of heterocyclic aryl vinyl ketones: Development of a cost-effective route to cyclization substrates. **H.A. Young**, W.L. Ashley, T.C. Coombs

CHED 1381. Development of iron-based hydrogenation catalysts: Applications in the pharmaceutical industry. **J. Mobley**, L. Boisvert

CHED 1382. Synthesis and characterization of meso-tetrakis(2-fluoro-6-methoxyphenyl)porphyrin. **A. Adeyemo**

CHED 1383. Synthesis of 6,24-tritriacontene-2-one, a brown tree snake pheromone. **A. Johnston**, S. Lewis

CHED 1384. Metal complexes of a new photosensitizer: Potential anticacer agent. **A. Adeyemo**

CHED 1385. Synthesis of a photoactivatable protecting group for biological thiol activation. **S. Fang**, **A.D. Fenton**, M.D. Distefano

CHED 1386. Characterization of diene degradation products from allylic tosylate elimination. **T. Lingo**, C. Paquin, D.W. Boerth

CHED 1387. Regioselectivity in nucleophilic aromatic substitution with aryl sulfonates. **F.N. Ngassa**, E. Bookout, Z. Patel

CHED 1388. Searching for chirality in a new route to heteroleptic alkylphosphine oxides. **A.L. Dixon**, J. Barry, D.R. Tyler

CHED 1389. Synthesis of quinone methide precursors as acetylcholinesterase reactivators. **S. Sillart**, C. Callam

CHED 1390. Nucleophilic atroposelective kinetic resolution of selective pyrrolopyrimidine kinase inhibitors. **T. Duong**, J. Gustafson, M.M. Cardenas, S. Toenjes, C.J. Nalbandian

CHED 1391. Expansion of tosylation on new allylic systems. **C. Sherlock**, C. Paquin, D.W. Boerth

CHED 1392. Fluorogenic polymerization amplification as a new platform for disease detection. **J. Sackey-Addo**, Z. Allen, M. Hopps, J. Anderson, D. Tahseen, C.B. Cooley

CHED 1393. Utilization of a variety of internal and termial alkynes toward a mercury-free, hydration reaction. B. Ide, C. Postel, **P.A. Shelton**

CHED 1394. Synthesis of espintanol analogues for the treatment of leishmaniasis. **S.P. Stokes**, G.R. Naumiec

CHED 1395. Microwave-assisted gold(I)-catalyzed Friedel–Crafts-like arylation of benzylic alcohols to afford 1,1-diarylmethanes. **J. Oakley**, T. Stanley, R.G. Iafe

CHED 1396. Synthesizing the 7-carbon analog of glucaric acid. **D.G. Abraham**, M. Hayes

CHED 1397. Design of hydrogen-bonded

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ternary cocrystals using a ditopic donor molecule and two acceptor molecules. **B. Mihelich**, D. Adsmond, R.J. Staples, S.M. Biros

CHED 1398. Evaluation of phenol modification in tandem Ugi-Smiles Diels-Alder reactions. **N. Revelt**, S. Luesse

CHED 1399. Investigation of the hydrogen bond connectivity between sulfa drugs and hydrogen bond acceptors in cocrystals. **I. Steinke**, D. Adsmond, K.A. Wheeler, R.J. Staples, S.M. Biros

CHED 1400. Iron-catalyzed reduction of Mannich bases. **K. Ferguson**, R.E. Whittaker, A. Redden

CHED 1401. Amide bond activation as an entry to alkene carboacylation. **J. Humke**, J. Walker, K. Vickerman, L.M. Stanley

CHED 1402. First steps towards fast and selective synthesis of substituted pyranones. **M.D. Ruane**, **J. Nawara**, **D. Hernandez**, **L. Terrill**, **F. Rueda**

CHED 1403. Development of a polymer-backed, regenerating chlorinating agent. **M.D. Ruane**, **F. Rueda**, **L. Terrill**, **D. Hernandez**, **J. Nawara**

CHED 1404. Synthesis of 2-(fluoromethyl)-phenol. **Z. Wei**, R.E. Rosenberg

CHED 1405. Fluorescence-based sensors for the detection of biologically relevant ions. **D.M. Schnable**, N. Edwards

CHED 1406. Synthesis and coupling schemes of naphthalimide compounds with target drugs. **K. Parrott**, J.E. Elbert, T. Divis

CHED 1407. Comparative studies of metal complexes of meso-tetrakis(2-bromo-3-hydroxy-4-methoxyphenyl) porphyrin. **A. Adeyemo**

CHED 1408. Synthesis of photochromic and fluorescent imines. **M.R. Berry**, J.T. Ippoliti

CHED 1409. Withdrawn

CHED 1410. Synthesis of alkenylthiols and their formation as self-assembled monolayers for use in the laccase-mediated removal of phenolic compounds. **A.R. Preciado**, C.M. Johnson, B.W. Gregory, P. Wiget

CHED 1411. Synthesis of porous polymer electrolyte films using a nanophase separation approach. **T. Ali Kizi**, L. Wang, D.C. Teeters, A.A. Lamar

CHED 1412. Activated carbon for urea adsorption. **L. Eickhoff**, B.J. Winters, K.E. Rohly

CHED 1413. Regio-selective hydrogen-deuterium exchange reaction. **A. Martinez**, T. Nguyen, **N. Chandra**, **E. Nevarez**, X. Chen

CHED 1414. Diaminonaphthalene derivatives for tuning the phase behavior of a photoconductive charge-transfer liquid crystal. **N. Smith**, J. Reczek

CHED 1415. Structural elucidation of pyrrolizidine alkaloids from *Buglossoides purpurocaerulea*. **C.J. Burghard**, **P.E. Plucker**, **S.M. Stroud**, **R.B. Kelley**

CHED 1416. 6-Methylpyrid-2-yl thio glycosides. **S. Hasty**, J.E. Scherer

CHED 1417. Exploration of nitrogen-tethered [5+2] oxidopyrylium-alkene based cycloadditions. T.A. Mitchell, **J.P. Grabowski**

CHED 1418. Atroposelective dynamic kinetic resolution of aryl-naphthoquinone ethers. A.N. Dinh, R. Noorbehesht, **A.C. Jackson**, J. Gustafson

CHED 1419. Activated carbon urea adsorption with auxiliary complexing agents, SDDC and NTA. **T. Riggs**, B.J. Winters, K.E. Rohly

CHED 1420. SuFEx based click chemistry for peptide stapling. **J. Han**, V.V. Fokin

CHED 1421. Acridone compounds in cancer research. **H.n. Fleegle**, D. Fish

CHED 1422. Organocatalyzed pericyclic reactions: Exploring catalyst reactivity and substrate scope. **E. Rivera**, A. Imanishimwe, H.A. Dahlmann

CHED 1423. Tenofovir: A novel approach using commercially available, inexpensive material. **E. Stryker**, H.P. Mangunuru, E. Yu, F. Gupton

CHED 1424. Synthesis of hyaluronic acid mimics for targeting CD44. **M.A. Vencil**, A.J. Krueger, M.L. Regan, E. Xu, K.E. Gonzalez, N.L. Snyder

CHED 1425. Mild catalytic method for sulfenylation of electron-rich aromatics. **E. Alvarez**, C.J. Nalbandian, J. Gustafson

CHED 1426. Kinetic & thermodynamic studies of 2-furylmethyl benzoate and 2-(methoxymethyl)furan in model Diels-Alder reactions. **J. Kosko**, W. Hollis, P.A. Deck

CHED 1427. Synthesis of pyrrolidinium-based poly(ionic liquids) and examination of their antibacterial properties. **K. Richey**, T.R. Hayden

CHED 1428. Potential candidate for the evaluation of hydrogen bonding: Attempted synthesis of 9-fluoro-9H-fluoren-1-ol. **M. Hanna**, R.E. Rosenberg

CHED 1429. Synthesis and studies of thiourea and amidothiourea based anion sensing receptors. **H. Hance**, M.O. Odago

CHED 1430. Supramolecular assembly of a sulfonated calix[4]arene with 1,4-diazabicyclo[2.2.2]octane derivatives. **H. Glick**, J.L. Fantini

CHED 1431. Investigating the reactions of zinc enolates in aqueous solutions. **I.C. Anderson**, W.E. Brenzovich

CHED 1432. Kinetic studies of model Diels-Alder reactions using ^{19}F NMR. **N. Price**, W. Hollis, P.A. Deck

CHED 1433. Investigation of the solvatochromic properties of benzo[c] fluorenone. **J. Napoli**, **R. Black**, T.C. Celius, B.W. Williams

CHED 1434. Triazole derivatives from 2-bromomethyl-3-phenylpyrazine. **L.M. Swanson**, A.M. Schoffstall

CHED 1435. Investigations into the effect of alkoxy substitution on palladium-catalyzed olefin difunctionalization. **M.C. Maust**, W.E. Brenzovich

CHED 1436. Synthesis of doxorubicin analogs for DNA binding studies. **H.M. Anchukaitis**, S.S. Tartakoff, S. Glazier

CHED 1437. Developing a flow process for a stereoselective aldol-spoxidation reaction. **D. Bell**, J.A. Hansen, K. Ruark, Y. Sawyer

CHED 1438. Determination of equilibrium constants of furan derivatives in model Diels-Alder reactions with *N*-(4-fluorophenyl)maleimide. **A. Corpuz-Nicolas**, W. Hollis, P.A. Deck

CHED 1439. Reaction schemes for the synthesis of photo-active naphthalimide-drug compounds. **T. Divis**, J.E. Elbert, K. Parrott

CHED 1440. Progress toward a calixarene–viologen unit for AB-type supramolecular assembly. **H. Tran**, J.L. Fantini

CHED 1441. Synthesis of perfluoropyridyl-1*H*-1,2,3-triazole derivatives. **M.N. Trujillo**, A.M. Schoffstall

CHED 1442. Withdrawn

CHED 1443. Synthesis of novel tripodal polymer frameworks based upon a 1,3,5-substituted aromatic ring. **B. Nagle**, T.A. Knoerzer

CHED 1444. Synthesis of novel aromatic heterocycles via oxo- and imino-gold carbene intermediates. **M. Marchioretto**, T.A. Knoerzer

CHED 1445. Stereodivergent syntheis of (+)- and (-)-pilosinine. **R.E. Anderson**, **T.J. Gibson**, R.J. Mullins

CHED 1446. Determination of phytosterols in dried shaggy mane and morel mushrooms by GC-MS. **N. Walker**, A. Overgard, S. Quint, T.W. Nalli

CHED 1447. Synthesis of isoxazoles via copper(I) catalysis with *N*-chlorosuccinimide. **W.R. Morris**, A.M. Schoffstall

CHED 1448. Mechanistic investigations into a novel palladium-catalyzed oxidative difunctionalization reaction. **Z.L. Croft**, W.E. Brenzovich

CHED 1449. Synthetic studies on guaipyridine alkaloids: Rupestines L and M. J.R. Vyvyan, **M. Deshaye**

CHED 1450. Triazole synthesis and microwave-assisted Diels-Alder cycloaddition. **J.L. Montanez**, A.M. Schoffstall

CHED 1451. Impact of water on lowering the catalyst loading in cobalt-catalyzed Kumada coupling reactions. **J.J. Mercado**, M.C. Perry

CHED 1452. Synthesis and isolation of functionalized quinoxalyltriazoles. **C.M. Clements**, A.M. Schoffstall

CHED 1453. Development of a fluorescent sensor for the detection of copper(II) and iron(III) ions. **A. Garber**, N. Edwards

CHED 1454. Sonogashira coupling reactions with bromomethyl quinoxaline derivatives. **A.T. McGrath**, **K.A. Stewart**, A.M. Schoffstall

CHED 1455. Synthesis of indolyl/indazolyl (N1 substituted) quinolones (C6 and C8 substituted) for study as possible anticancer/antibiotic/antimicrobial agents: Desired cyclized product or uncyclized intermediate? **K.R. Reicher**, **K.J. Derkson**, **R.A. Heyblom**, **M.A. Johnson**, **H.L. Carlson**, J. Thomforde, M. Msaki, L.M. Ito, P.G. Schulzetenberg, D.A. Luke, **J.L. Langer**, **H.R. Olson**, R.R. Hansen, N. Beaulieu, **A. Davidson-Hunt**, T.M. Trygstad

CHED 1456. Computational studies of 1,2-diols. **L. Metoyer**, **D. Mbunwe**, J. Armstrong, K. Jenkins, K.M. Morgan

CHED 1457. Novel synthesis of serotonin using relatively mild reagents. **T.J. Oleskey**, K.M. Halligan

CHED 1458. Tertiary benzamides as possible antimalarial leads. **E. Williford**, M.J. Campbell

CHED 1459. Synthesis of phenol and pyridine containing LOX inhibitors. **P. Patel**, **F. Cervantes**, **F. Ramirez**, **A. Wan**, D.M. Solano

CHED 1460. Copper-catalyzed silylations of C—C π-bonds. **S. Harruff**, B.K. Mikesell, R. Van Hoveln

CHED 1461. Synthesis of oxobutanoate-substituted carvacrol and thymol derivatives as potential antibacterial agents. G.E. Henry, **A. Graybill**, N. Brotzman, A. Cocolas

CHED 1462. Synthesis and biological activity investigation of acetylphenyl benzoates. **R. Potenzino**, L. Chablani, R.N. Manchanayakage

CHED 1463. Synthetic studies on cananodine: Setting the C8 stereocenter. **R. Sabio**, J.R. Vyvyan

CHED 1464. Disilylation of aldehydes and ketones using a copper catalyst. **B.J. McCarty**, **W.L. Kirkman**, R. Van Hoveln

CHED 1465. Homocoupling of alkyl and vinylboronic acids using Mn(III) compounds: A first look. **Z.A. Kohanov**, C.E. Harris

CHED 1466. Copper-catalyzed nucleophilic addition to carbonyls using organosilanes. **T.S. Carpenter**, **B.M. Thomas**, R. Van Hoveln

CHED 1467. Design and synthesis of an effective tridental molecular receptor for fullerenes. **M. Kramer**, C. Lee, M. Perkins, C. Griffin, P.A. Denis, M. Yanney

CHED 1468. Investigations into ligand tunability: Synthesis and characterization of NS containing cryptands. **L.M. Sadlowski**, T.L. Walker, I. Taschner

CHED 1469. Drug repositioning and diversification strategy for discovery of compounds with anti-cancer activity. **D. Gibson**, **M. Chapa**, B.A. Rowland, D. Bateman

CHED 1470. Design and synthesis of triphenylene based molecular receptors for fullerenes. **C. Lee**, C. Griffin, P.A. Denis,

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M. Yanney

CHED 1471. Exploring the use of both planar and curved Surface polycyclic aromatic hydrocarbons in the design and synthesis of molecular receptors for fullerenes. **C. Griffin**, C. Lee, P.A. Denis, M. Yanney

CHED 1472. Chemical composition of an acetone extract of *Vitis riparia*. **G.D. Reynolds**, J. Yarger, E. Castner, A. Graybill, G.E. Henry

CHED 1473. Selective functionalization of the primary rim of alpha-cyclodextrin for practical applications. **J.A. Romo**, O. Bistri, M. Sollogoub

CHED 1474. Conversion of ureas to hydroxyguanidines for conjugation to drug-releasing polymers by nitroso-Diels-Alder reactions. **N.G. Foulon**, M.N. Radford, N.A. Yakelis

CHED 1475. Microwave-assisted hydrogenations using frustrated Lewis pairs. **Y. Miao**, L. Robertson, E.M. Valentin

CHED 1476. Ionic salts of juglone for herbicidal applications. **I.L. Crouch**, T.W. Majors, O.A. Cojocaru

CHED 1477. Synthesis and structural characterization of thiophene-fused aza-BODIPY dyes. **C.R. Youshaw**, D. Chase

CHED 1478. Synthesis of secondary amides from amine derivatives and propionitrile using a continuous flow process. **K. Larson**, M.T. Wentzel

CHED 1479. Small molecular study of the dynamic exchange of the thiol-Michael reaction. P. Chakma, B. Zhang, **Z. Digby**, D. Konkolewicz

CHED 1480. Synthesis and NMR characterization of new isatin sulfonic acid thiosemicarbazone compounds. **C.E. Methvin**, E. Rush, E.C. Lisic

CHED 1481. Synthesis and photophysical properties of distyryl β–ketoiminate boron difluoride complexes. **L. Stevens**, C. Moore, D. Chase

CHED 1482. Synthesis and reactivity of (phenyliodonio)pyridines: Reagents for pyrdinylation of nucleophiles. **R. Novak**, M.W. Justik

CHED 1483. Synthesis and biological evaluation of caffeic acid phenethyl ester (CAPE) derivatives as xanthine oxidase inhibitors. **S. Onate**, H. Istre, B. Heppler

CHED 1484. Organocatalytic synthesis of N,O-acetals by C–N bond insertion of aldehydes into electronically-activated amides. **T. Wittman**, M. Paeth, C. Rickerman, P. Willoughby

CHED 1485. Withdrawn

CHED 1486. Modified click-style Sonogashira coupling reactions involving silyl-protected alkynes at room temperature. **M.J. Mio**, S.M. Brikho, K. Suiter, M.M. Payne, H. Ali, N.R. Boynton, M.T. Dickow, P.S. Kamash, B.M. Ross, C.N. Sayah, S. Sayed

CHED 1487. Gem-dimethyl moiety β to hydroxyl position promotes cyclooctanoid synthesis via tandem 6-exo dig cyclization/Claisen rearrangement. **W.C. DeLomba**, T.V. Ovaska

CHED 1488. Exploring the effects of a nitro group and lateral methyl groups on the phase behavior of 1-3-4-oxadiazole-based liquid crystals. **M. Riley**, E. Scharrer

CHED 1489. Salt formation vs. co-crystallization: An exploration of the ΔpK_a rule for a series of aromatic acids and bases. **K. Powers**, D.K. Geiger

CHED 1490. Synthesis of thujone derivatives as potential antibacterial agents. G.E. Henry, **E. Castner**

CHED 1491. Intramolecular spiroether synthesis from peroxy enolates. **L. Fan**, K.T. Kuwata

CHED 1492. Synthesis of tetrahydroquinoline derivatives as novel histamine H_4 receptor antagonists. **H. Cheung**, A. Clark

CHED 1493. Synthesis and characterization of novel unsymmetric dithiocarbamate ligands. **R. Blumling**, M.E. Railing

CHED 1494. Synthesis of a nitrogen containing cyclooctanoid structure via tandem 6-exo dig cyclization/Claisen Rearrangement. **N.M. Theopold**, T.V. Ovaska

CHED 1495. Synthesis and NMR analysis of PPDO-TSC and INAP-TSC compounds: Complexation to form their Cu(II) complexes. **G.L. LaSala**, E.C. Lisic

CHED 1496. Synthesizing amines using cyanates and carbamates. **K. Marzotto**, B. Linton

CHED 1497. Design and synthesis of asymmetric ferrocenyl-substituted *N*-heterocyclic carbenes. **K. Freshour**, M.O. Odago

CHED 1498. Thermal chemistry of spiro[bicyclo[4.2.0]oct-2-ene-7,1′ –cyclopropane]. **Y. Zhang**, P.A. Leber

CHED 1499. New rosin materials for the delivery of pharmaceuticals in liquid form. **J. Scantland**, O.A. Cojocaru

CHED 1500. Exploring new unsymmetrically substituted oxadiazole-based liquid crystals: Optimization of the synthetic approach and phase behavior. **B. Bordokas**, A. Lisovsky, E. Scharrer

CHED 1501. Synthesis of new AMPY thiosemicarbazone ligands to form their respective Pd(II) metal complexes. **J.D. DeVaney**, W.G. Qualls, W. Carroll, E.C. Lisic

CHED 1502. Synthesis and NMR characterization of chloro-isatin thiosemicarbazone compounds. **J.E. Little**, A.K. Buckner, E.C. Lisic

CHED 1503. Utilization of spent coffee grounds for purification of biodiesel. **K.D. Dema**, J. Leake

CHED 1504. Effects of poor nutritional habits on the active ingredients in oral rinses. **J.O. Graham**, K.M. Halligan

CHED 1505. Synthesis, purification and characterization of the 2-selenylimidazole analog of L-histidine. **A. Schroll**, J.J. Dyer

CHED 1506. Effects of structural variation on aryl aldimine basicities. **N. Capra**, J. Bennett

CHED 1507. Tuning the recognition of biological phosphates by modifying the anion recognition group on a synthetic receptor. **S. Wakefield**, **H.C. Adamson**, K.J. Clear

CHED 1508. Quantification of ethanol in beverages using ^{1}H NMR. **M.D. Kellner**, J. Bennett

CHED 1509. Replacing liquid:liquid extraction: The use of swellable organically modified silica for the purification of organic compounds. A.N. Whitesell, **N.N. Shaw**, H.K. Huston, J.R. Hinds, E.B. Vaughan

CHED 1510. Synthesis and evaluation of the catalytic activity of a (cyclopentadienone)iron tricarbonyl compound in oxidative and reductive transformations. **E.E. Harrison**, T.W. Funk

CHED 1511. Effect of chain length on gelation ability of several biphenyl long-chain diesters. **S. Moore**, J. Schulman, M. Tran, C. Geiger

CHED 1512. Apocynin as an NADPH oxidase inhibitor. **T. Welsch**, J. David

CHED 1513. Green dehydrations for the undergraduate organic chemistry laboratory. **J.L. Terry**, M.S. Erickson

CHED 1514. Sonicated Mitsunobu reaction: Using the kinetic isotope effect for mechanistic analysis. **A. Intelli**, **M. Vukicevich**, M. Furgione, M. States, R. Heckler, R. Florre, S. Rajaraman, P.G. Cohn

CHED 1515. Withdrawn

CHED 1516. PEG-Stapled peptides: A novel stabilization method. **N. Brown**, Q. Xiao, J.L. Price

CHED 1517. Gold-catalyzed reactions of epoxy esters. **E. Starchman**, C. Enciso, J.R. Vyvyan

CHED 1518. Investigation of long-wavelength, photocleavalbe protecting groups based on nile red. **E.R. Ranney**, T.C. Celius

CHED 1519. Development of a dye displacement assay for the evaluation of aldol catalysts. **E. Aguiluz**, L. Witus

CHED 1520. Using rosin based ligands to bind transition metals. **R.H. Hall**, O.A. Cojocaru

CHED 1521. *N*-Substitution of carbazole centered ligands for metal binding applications. **K. Schofield**, A. Brown

CHED 1522. Synthesis and characterization of alkyl-pyrophosphate donors for the chemoenzymatic diversification of natural products. **J. Masterson**, **C. Bandari**, E.M. Scull, R.H. Tran, S. Singh

CHED 1523. Separation and analysis of the products from the reaction of 3-methyl-1-phenyl-2-pyrazoline-5-one and furfural. **A. Serreyn**, J.C. Easdon

CHED 1524. Quantum mechanical investigation of novel Friedel-Crafts acylation products. **A.M. Dove**, W.M. Ames

CHED 1525. Functionalization of polyacrylates with TEMPO, PEG and hemoglobin binding groups. **M.E. Michaud**, O. Alomainy, A. McMahan, N. Singleton, H.J. Schanz

CHED 1526. Oxidation of secondary aromatic alcohols. **S.W. Baer**, **H. Jia**, L. Farber

CHED 1527. Synthesis and characterization of β-substituted chalcones and alkenones. **E. McClure**, L. Dolph, S.R. Sieck

CHED 1528. Synthesis and spectroscopic characterization of naphthalic anhydride derivatives. **E.C. Olson**, C.H. Battle

CHED 1529. Using the ionic liquid strategy to prevent drug-induced liver injury. **S. Visneski**, O.A. Cojocaru

CHED 1530. Towards the synthesis of crassalactone A and development of hetero Diels-Alder methodology to access styryl lactones. **R. Hippman**, J.A. Mueller

CHED 1531. Rapid synthesis of *N*-(10-chloro-9-anthrylmethyl)-*N*-methylformamide. **J. Gooding**, L.I. Bobyleva, M.M. Bobylev

CHED 1532. Studies towards the synthesis of lobophorol derivatives. E.M. Valentin, **S. Hackenburg**

CHED 1533. Synthesis and characterization of fluoreno[3,2-*b*] fluorene derivatives. **V.A. Larson**, J.E. Barker, L.N. Zakharov, M.M. Haley

CHED 1534. Copper-catalyzed approach to beta-lactams. **M. Chaoui**, A.K. Isaacs

CHED 1535. Imine library synthesis via solvent-free reactions. J.E. Thames, S.K. Gillis, **S.M. Kennedy**

CHED 1536. Conformational analysis of β-substituted chalcones. **R. Xia**, T.A. Mobley, S.R. Sieck

CHED 1537. Thermal chemistry of 7-alkybicyclo[3.2.0]hept-2-enes. **K. Kidder**, P.A. Leber

CHED 1538. Ammonia-borane as a hydrogen source for the reduction of amides to amines under mild conditions. **E. Pappaterra**, H. Dai, H. Guan

CHED 1539. Convenient synthesis of a dicyanoacetylene equivalent: Useful precursor to tetraazaporphyrins. **J. Korenak**, **J.P. Fitzgerald**

CHED 1540. Enantioselective catalysis using chiral Ti-Pd complexes. C. Ence, W. Walker, **E. Martinez**, D. Michaelis

CHED 1541. From detection to complexation: Detecting and removing aluminum from aqueous solutions. J.P. Ricket, J. Bowlin, **M.W. Fultz**

CHED 1542. Design, synthesis, and evaluation of cyanine-like fluorescent dyes for use as surgical tracking and visualization tools. **A.M. Noyes**, V.K. Dunlap

CHED 1543. Effects of adding a biguanide to carbohydrates on blood

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glucose reabsorption. **C. Harmon**, J. Chaytor

CHED 1544. Enantioselective cross aldol reactions of aldehydes. **C. Slone**, B.G. Vanness

CHED 1545. Synthesis optimization and applications of a chiral selector adsorbent. **M. Dong**, S.A. Henrie

CHED 1546. Evaluating the potential of DPA to bind calcium, strontium, and barium cations from hydraulic fracturing flowback water. A.K. Merrill, **R.M. Moyles**, S.G. Tajc

CHED 1547. Squaramide-based anti-parasitic drugs toward the discovery of novel treatments for American trypanosomiasis. **E.N. Tran**, G.R. Naumiec

CHED 1548. Progress towards amino diversification of thiol phosphonamidates. **M. Bidzimou**, S. Bruhn, S.R. Sieck

CHED 1549. Synthesis of a cavitand for use in eight-helix template assembled synthetic protein systems. **J. Delegard**, N.A. Yakelis, J. Freeman

CHED 1550. Synthesis of dianthin G, a peptide that promotes the formation of osteoblasts. **K. Underwood**, N. Toupin, P. Fryfogle, J. Chaytor

CHED 1551. Synthesis and characterization of novel metal-organic frameworks for the destruction of chemical warfare agents. **C. Whitaker**, P. Brennan, T. Hentges

CHED 1552. Synthesis of 2-dimensional aminopolyphenylethynylarenes. **B. Holmes**, T.D. Selby

CHED 1553. Proposed synthesis of anomoian B. **A. Merry**, K. Chan, N.Y. Stessman

CHED 1554. Investigation of electronic variables of x-pyrone-based oxidopyrylium-alkene [5+2] cycloadditions. **J. Shaw**, T.A. Mitchell

CHED 1555. Carbodiimide approach to the synthesis of chiral alpha-amino ester sulfinamides. **S. Waggoner**, S.R. Hitchcock

CHED 1556. Synthesis of 2-dimensional polypyridinylethynylarenes. **R.S. Ruiz**, T.D. Selby

CHED 1557. Investigation of chemoselective benzylic oxidation transforming toluene into benzaldehyde. **C. Carroll**, L. Handlin, B. Sweetman, Y. Liu

CHED 1558. Development of a greener method for modifying silica gel with a dendritic precursor for chiral column chromatography. **A. Forderhase**, S.A. Henrie

CHED 1559. Synthesis of 2-dimensional polyphenylethynylarenes. **K. Harthcock**, L. Bicker, T.D. Selby

CHED 1560. Synthesis of tropone-fused porphyrins. **E.K. Cramer**, T.D. Lash

CHED 1561. Michael reactions of tropone iron tricarbonyl: Towards the synthesis of complex azapolycycles. D. Griffith, **S. Valent**, **R. Tritt**

CHED 1562. Intramolecular 1,3-dipolar cycloaddition of a nitrone to a 1,4-quinone. **S.K. Bentley**, W.G. McMahon

CHED 1563. Synthesis of 2-dimensional polyphenylbuta-1,3-diynylarenes. **M. Martin**, T.D. Selby

CHED 1564. Synthesis of indenopyrazole and dihydroindenopyrazole compounds as potential pharmaceuticals. **C. Sullivan**, D. Stanley, F. Peters, M.T. Blankenbuehler

CHED 1565. Organic synthesis of *O*-acylated amino acid surfactants to examine antibacterial properties. **A. Szczepanski**, D.M. Tobiason, F.H. Billiot, D. Brownholland

CHED 1566. Palladium-catalyzed direct β-heteroarylation of ketones: Unusual domino reaction discovery. **Q. Nguyen**, S. Costan, A. Quillen, L. Ma

CHED 1567. Solid state energy transfer in multi-chromophore thin films of quinolate and BODIPY. J. Vaal, D. Eble, J. Acchiardo, K. Boggavarapu, **P. Hewavitharanage**

CHED 1568. Design and synthesis of triazole containing PNA monomers capable of triplex formation with the A-U base pair in double-stranded RNA. **A.K. Williams**, E. Rozners, J.A. MacKay

CHED 1569. Silica gel supported oxidative cleavage of alkynes using a ruthenium tetroxide catalyst. **H. Thompson**, M. Ali, R.A. Ripa

CHED 1570. Why are Hammett constants so effective in predicting the non-covalent binding energies of aromatic interactions: A review. J. Carey, M. Roguski, **D.A. Engebretson**

CHED 1571. Preparation and NMR analysis of chalcone derivatives. **A. Zeng**, T. Sapienza, M. Young

CHED 1572. Phosphine-free palladium catalysts for the direct arylation of heterocyclic aromatic compounds. **C. Franklin**, S.A. Alaniz, K.H. Shaughnessy

CHED 1573. Protein phosphatase inhibitors: An analysis of functionality, placement, and stereochemistry. D. Forbes, **L. Lopansri**, M. Forbes, H. Bobinger

CHED 1574. Evaluation of long-range hyperconjugation in constrained eight-membered rings. **J. Walters**, B. Bashrum, G. dos Passos Gomes, P. Wiget

CHED 1575. Continuous flow synthesis of quinones. **K. Volpe**, E.E. Podlesny

CHED 1576. Discovery of antibiotic compounds from natural ecological interactions of marine bacteria. **K.M. Greskovich**, S. Mascuch, J. Kubanek

CHED 1577. Synthesis and characterization of porphyrin and bacteriochlorin based gylcoconjugates. **M.R. Parris**, **N. Abualeinan**, M.C. Bennion, A. Henderson, D. Dennis, M. Burch, N.L. Snyder, **J.V. Ruppel**

CHED 1578. Flow synthesis of an epoxide and brine shrimp lethality assay. **E. Grubbs**, J.A. Hansen, K. Panos

CHED 1579. Prodrug syntheses of an inhibitor of the deoxyxylulose reductoisomerase (DXR): A potential new antitubercular drug. **I.M. Manning**, M. Munier, D. Lievremont, C. Grosdemange-Billiard

CHED 1580. Rapid synthesis of *N*-methyl-*N*-(4-nitrobenzyl)formamide. **E.A. Hernandez**, L.I. Bobyleva, M.M. Bobylev

CHED 1581. Synthesis and preliminary aqueous kinetic studies of carbinolamides derived from ketones. **R. Epplin**, A.L. Heinold, M. Dalton, R.W. Nagorski

CHED 1582. Progress toward the total synthesis of lauroside B. **V. Lansdale**, G.M. Smith

CHED 1583. Rapid Synthesis of *N*-(3-fluorobenzyl)-*N*-methylformamide. **T.A. Skinner**, L.I. Bobyleva, M.M. Bobylev

CHED 1584. Mechanochemical synthesis of diphenylporphyrins. **M. Reyes**, A. Henderson, J.V. Ruppel, T.D. Hamilton

CHED 1585. Rapid synthesis of *N*-methyl-*N*-(2-trifluoromethylbenzyl)formamide. **T.A. Dostert-Azzarello**, L.I. Bobyleva, M.M. Bobylev

CHED 1586. Synthesis of stabilizing ligands for metal oxide nanoparticles. **E. Agwaramgbo**, Y.A. Tran, V.L. Kolesnichenko, G.Z. Goloverda

CHED 1587. Enhancing an oxidation experiment. N.J. Beyer, **V.J. Henry**, **E.J. Popma**

CHED 1588. Synthesis of LpxC substrate analogs for antibiotic. **W. Clay**, B. Lewis, A. Jagger, R.L. Woodward

CHED 1589. Synthesis of generation 3-bisMPA dendrimers for nanotherapeutic drug delivery systems. **G. Hodge**, J. Manono, S.C. Dimaggio

CHED 1590. Retro-Diels-Alder reactions of nitrosocarbamimides as potential urea prodrugs. **N.T. Tran**, N.A. Yakelis

CHED 1591. Synthesizing polyhydroxylated indolizidines from D-glucopyranoside. **S. Bryson**, L.J. Liotta

CHED 1592. One-pot preparation of 2,7-disubstituted cycloheptanones and their ring-closing metatheses. N. Behrens, A. Yoon, **J.B. White**

CHED 1593. Investigations into the conjugate hydrocyanation of α,β-unsaturated aldehydes in organic synthesis. **V. Nguyen**, M. Hubbuck, W. Serrano, T. Black, K. Carey, N.C. Kallan

CHED 1594. Mechanisms of flavin cofactors for enzymatic function. **M.A. Smith**, A.W. Jensen, D.K. Mohanty, W.L. Dilling

CHED 1595. Rapid synthesis of *N*-methyl-*N*-(3-nitrobenzyl)formamide. **M.D. Rodgers**, L.I. Bobyleva, M.M. Bobylev

CHED 1596. Synthesis, characterization, and phototoxicity studies of novel paraben compounds. **C. Alderman**, K. Pate, K.S. George Parsons

CHED 1597. Rapid synthesis of *N*-methyl-*N*-(4-phenylbenzyl)formamide. **M. Gudejko**, L.I. Bobyleva, M.M. Bobylev

CHED 1598. Visible light-induced regioselective remote halogenation of 1,2-diaminobenzene derivatives. **C.R. Smith**, D. Reddy, E. Watkins

CHED 1599. Chemo- and regioselectivity of hydroxyl radical reactions with arenes: How important is hydrogen abstraction? **A. Waggoner**, E.P. Gibson, M.A. Buckles, J.S. Poole

CHED 1600. Rapid synthesis of *N*-(9-anthrylmethyl)-*N*-methylformamide. **K.H. Heick**, L.I. Bobyleva, M.M. Bobylev

CHED 1601. Organic dye, visible-light photocatalytic imidation of arenes using *N*-halo reagents. **F.H. Refai**, D. Rogers, C.A. Cantwell, A.A. Lamar

CHED 1602. Synthesis of 1,2-dihydroisoquinolines. **J. Hendsey**, **J. Nicholson**, A.K. Isaacs

CHED 1603. Retro-nitroso-Diels-Alder reactions of 1-substituted-1,3-cyclohexadienes as a strategy for long-acting drug-polymer conjugates. **M.J. Kim**, J. Wong, N.A. Yakelis

CHED 1604. Modifications to *para*-menthane-(3,8)-diol to increase mosquito repellency. **H. Nowakowski**, C.M. Taylor

CHED 1605. Process development of a quinone-aldehyde synthesis for the purpose of studying intramolecular 1,3-dipolar cycloadditions. **A.N. Connolly**, W.G. McMahon

CHED 1606. Microwave synthesis of tetraphenylporphyrins and tetraphenylporphyrin derivatives. E.A. Nalley, **C. Caveny**, P. Hyolmo, K. Vajgrt

CHED 1607. Synthesis of multi-modal drugs toward treatment of Chagas disease. **R.M. Senn**, G.R. Naumiec

CHED 1608. Rapid synthesis of *N*-(2-fluorobenzyl)-*N*-methylformamide. **H.S. Lee**, L.I. Bobyleva, M.M. Bobylev

CHED 1609. Aqueous fluorogenic polymerization for signal amplification. **Z. Allen**, J. Sackey-Addo, C.B. Cooley

CHED 1610. Isolation of saturated pyrrolizidine alkaloids from *Arnebia pulchra*, *Lindelofia anchusioides*, and *Omphalodes verna*. **J.D. Jacobs**, **L.K. Johnson**, **R.A. Davis**, **B.E. Schroeder**, **R.B. Kelley**

CHED 1611. Sulfonamide nucleosides: Synthesis and *in vitro* studies. **H. Jacobs**, **M. Mabry**, A. Awad

CHED 1612. Total synthesis of (+)-bovidic acid. **W.R. Cassels**, K.J. Quinn

CHED 1613. Development of strategies for the synthesis of benziporphyrin dimers. **R.A. Tomlovich**, T.D. Lash

CHED 1614. Synthesis of organic ligands for improving the behavior of luminescent solar concentrators. G. Ferguson, **R.C. Chambers**

CHED 1615. Palladium-catalyzed direct α-heteroarylation of ketones: Ketone substrate scope study. **K. Lindsay**, L. Ma, M. Neiser, A. Quillen, A. Rosen, S. Ramirez, Q. Nguyen

CHED 1616. Using ionic liquid strategy

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to convert phenothiazine drugs to a liquid form. **L. Pipkin**, O.A. Cojocaru

CHED 1617. Structure-activity studies in the pair-inclusion motif for peptide recognition by cucurbit[8]uril. **H. Taylor**, Z. Hirani, A. Bockus, E. Babcock, E. Boms, A.R. Urbach

CHED 1618. Synthesis of a divinylic carbaporphyrin for investigations into Diels-Alder cycloaddition reactions. **A.B. Carroll**, T.D. Lash

CHED 1619. Design and synthesis of an optically active ligand for the asymmetric preparation of non-proteinogenic amino acids. **K. Shoff**, T.K. Ellis

CHED 1620. Rapid synthesis of *N* -(4-fluorobenzyl)- *N* -methylformamide. **S. Park**, L.I. Bobyleva, M.M. Bobylev

CHED 1621. Reactions of imines with Danishefsky's diene. **C. Waters**, **D.P. Predecki**

CHED 1622. Optimization of reaction conditions for a visible-light photocatalyzed bromination of arenes using an organic dye. **R.G. Brown**, A.A. Lamar

CHED 1623. Synthesis of amino acids via diazo keto ester transformation. **N.A. Weirath**, **M. Bryan**, M.A. Lnu

CHED 1624. Dihydroxylation and alkene migration studies en route to altersolanol P. **B.L. Frey**, S.M. Kennedy

CHED 1625. Ugi-Smiles based triazole formation and derivatization. **H. Sperry**, S. Luesse

CHED 1626. Investigation of the role of light in the visible-light photocatalyzed activation of *N*-halosuccinimide reagents. **E.Y. Ko**, M.D. Hopkins, A. Lignieres, A.A. Lamar

CHED 1627. Progress towards the synthesis of the resin merremin E. **D. Schultz**, R. Ulrich, A. Pirinelli

CHED 1628. Solubility effects of sidechain modification in poly(phenylene vinylene) derivatives for use in organic light-emitting diode (OLED) devices. **G. Benito**, E. Evans, C.A. Young

CHED 1629. First survey of solution-state carbon-13 NMR spectra of ambers. **T.A. Contreras**, J.B. Lambert

CHED 1630. Synthesis of the isoindolinone moiety of stachybotrin D: Incorporating greener methods. **K. Alexander**, D.C. Bromfield-Lee

CHED 1631. Synthesis of amine conjugated naphthalimide derivatives. **G. Holtzman**, C.H. Battle

CHED 1632. Chlorination of heteroarenes under non-acidic, visible-light photoredox catalytic conditions. **J.C. Su**, A.T. Espinosa, D. Rogers, A.A. Lamar

CHED 1633. Synthesis and characterization of aza-Diels-Alder products. **B. Hockenberry**, **D.P. Predecki**

CHED 1634. Synthesis of covalently-linked fluorescent dye derivatives. **L. Pferdmenges**, K. Fogarty, P. Lundin

CHED 1635. Progress towards efficient synthesis of morphine analogue using the Wagner-Jauregg reaction. **A. Buck**, S.S. Tartakoff

CHED 1636. Oxidative addition of *para*-substituted aryl electrophiles to predict reaction selectivity. **A. Tomczyk**, A.K. Cooper, D.J. Nelson

CHED 1637. Reactions of acetophenones with nitric acid: The effect of ring substitution on β-nitration versus electrophilic aromatic substitution. **H. Tarbox**, N. Wachter

CHED 1638. Expanding the green scope of pentaerythritol acetal formation. J.R. Marrazzo, S.N. Simon, **S.M. Kennedy**

CHED 1639. Multivalent recognition of distant peptide sites by cucurbit[7]uril. **C. Kodadek**, A. Karla, Z. Hirani, H. Taylor, A.R. Urbach

CHED 1640. Utilization of the Thorpe-Ingold effect to access ketal- and dithioketal-functionalized cyclooctanoids via tandem 6-*exo* dig cyclization-Claisen rearrangement. **K.A. Alley**, T.V. Ovaska

CHED 1641. Selectivity of Wohl-Ziegler brominations of cyclohexene and *trans*-2-hexene. **R. Dorn**, T.W. Nalli, E. Willcox, J.K. West

CHED 1642. Synthesis of cyclized pharmaceutical precursors via activation of renewable sugars. **T. Schweickart**, J.A. Dabrowski

CHED 1643. Synthetic studies on brevicomin. **W.F. Connors**, **L.M. Howard**, K.J. Quinn

CHED 1644. Selective reactions of cysteine perflouroaryl thioethers. **A. Resnikoff**, J. Gavenonis

CHED 1645. Epoxidation studies of intermediates en route to altersolanol derivatives. **T.C. Bentzel**, S.M. Kennedy

CHED 1646. Development of synthetic method for the preparation of sulfinate esters and sulfinamides that minimizes the formation *S*-(*p*-tolyl) *p*-tolylthiosulfonate. **E. Jacobsen**, S.R. Hitchcock

CHED 1647. Exploring the regioselective Diels-Alder reaction scope of 1,4-naphthoquinones. **G.N. Good**, **W. Ma**, S.M. Kennedy

CHED 1648. Design and synthesis of oxadiazinones as tools for asymmetric organocatalysis. **T. Lindvall**, S.R. Hitchcock

CHED 1649. Isolation and elucidation of novel pyrrolizidine alkaloids from *Cryptantha maritima*. **B.L. Stavaas**, **M.M. Gianandrea**, **E.J. Holeman**, **R.B. Kelley**

CHED 1650. Coupling methods for 2,2′-bipyridines as precursors for novel Ru-bipyridine complexes. **A.R. Pasnon**, **S.B. Vazquez**, **B. Aukszi**

CHED 1651. Synthesis and evaluation of pyridine based quinone methide precursors for aged acetylcholine esterase reactivation. **J. Tabbaa**, A. DeYong, Q. Zhuang, A.J. Franjesevic, C. Callam, C.M. Hadad

CHED 1652. Synthesis and characterization of meso-tetrakis(5-fluoro-2-methoxyphenyl)porphyrin. **A. Adeyemo**

CHED 1653. Synthesis of hypophosphite esters using transesterification and the primary alcohol dodecanol and nonanol. **E. Shokoya**, S. Deprele

CHED 1654. Synthesis of methoxytetrahedrane and trimethylsilylbicyclobutane. **E. Hickey**, L.J. Tilley

CHED 1655. Synthesizing tetrahydroxylated indolizidines from L-glucose. **M. Pomfret**, L.J. Liotta

CHED 1656. Synthesis of pyridyl and propiolyl bicyclobutanes. **G.J. Giardino**, L.J. Tilley

CHED 1657. Synthesis of ergosta-5,22,24(28)-trienol. **C. Hilger**, T.W. Nalli

CHED 1658. Synthesis of sulfur- and nitrogen-containing constrained eight-membered rings for the evaluation of long-range hyperconjugation. **R.E. Lee**, B. Bashrum, G. dos Passos Gomes, P. Wiget

CHED 1659. Effects of alkyl substituents on the kinetics of beta-keto acids decarboxylation in aqueous solutions. **M. Springer**, A. Ignatchenko, W.W. Brennessel

CHED 1660. Synthesis of rasagiline and its derivatives. **T.S. Stercho**, J.K. Vohs

CHED 1661. New approach to the synthesis of 1,4-dithianes. **J.H. Oh**, F. Robertson

CHED 1662. Withdrawn

CHED 1663. Synthesis of amino alcohols from an epoxide. **A. Yu**, J.A. Hansen

CHED 1664. Lewis acid mediated synthesis of sulfonamides from sulfonyl fluorides. **C. Woroch**, M. Rusznak, C. am Ende, P. Mukherjee, R. Franzese, S. Etuk, S. Kwan, N.D. Ball

CHED 1665. Expedient method to fused sulfur-containing heterocycles. **E. Frisco**, F. Robertson

CHED 1666. Syntheses of laurencione and its derivatives: Is laurencione involved in bacterial communication?. **M. Dunbar**, D. Lievremont, C. Grosdemange-Billiard

CHED 1667. MacMillan-type Diels-Alder reactions using PAMAM bound imidazolidinone organocatalysts. **H.N. Koenig**, J.H. Ennist, M. Cloninger, T.N. Jones

CHED 1668. Nucleophilic aromatic substitution: Using microwave chemistry. **A. Madison**, K. Moore, N.H. Tran, L. Winfield, F.L. Payton

CHED 1669. Palladium-catalyzed direct β-heteroarylation of ketones: Reaction condition optimization. **A. Quillen**, Q. Nguyen, M. Neiser, A. Rosen, K. Lindsay, S. Ramirez, L. Ma

CHED 1670. Formation of peptide isosteres via olefin cross-metathesis. **T. Chickering**, B.R. Sculimbrene

CHED 1671. Quantum calculations of bimolecular etherification reaction of trifluoromethyl peroxides and Grignard reagents. **M. Kim**, K.T. Kuwata

CHED 1672. Hydrogen bonding of leaving group correlation to stereoselective outcome. **K.N. Bluhm**, **S. Easley**, S. Hasty

CHED 1673. Synthesis of *N*-(2,6-dimethylphenyl)-*N*-(2-formylphenyl) formamide. **R. Kutzner**, G. Nocera, J.A. Murphy

CHED 1674. Investigation of 4,2′pyridine-2-mercaptopyrimidine glycosides. **T. Nolkemper**, **J. Holbrook**, S. Hasty

CHED 1675. Two-step synthesis of complex aryl phosphonates via sequential elimination and 1,3-dipolar cycloaddition. **A. Haugen**, M. Schmid, E. Isaacson, J. Scanlon, P. Willoughby

CHED 1676. Historical pigments: Expanding scope, increased possibilities. **C. Knapp**, J.F. Lomax, S.Q. Lomax

CHED 1677. Aminoglycoside modification: The halogenation of kanamycin A. **S. Moore**, **S.E. Bowman**, A.L. Norris, E.H. Serpersu, D.C. Baker

CHED 1678. Intramolecular 1,3-dipolar cycloaddition of an azidoquinone. **C.A. McCabe**, W.G. McMahon

CHED 1679. Investigation of oxygen tethered pyrones toward [5+2] cycloadditions. T.A. Mitchell, J.R. Goodell, **J. Bulandr**

CHED 1680. Synthesis and reactivity of a variety of 1-aroyldiaziridine derivatives. **L. Ostopowicz**, **C. Nowak**

Section H
ErnestN. Morial Convention Center
Halls D/E

Undergraduate Research Posters

Physical Chemistry

Cosponsored by SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 1681. Investigating computational methods to predict organic redox potentials. **T. Rivera**, B. Levine, D. Hardwick

CHED 1682. Effects of molecular changes on verdet constants of achiral organic solvents. **G. Cifelli**, J. Orr

CHED 1683. Gas-phase spectra of MgO molecules: Possible connection from gas-phase molecules to planet formation. **K. Kloska**, R.C. Fortenberry

CHED 1684. Kinetic analysis of supported lipid bilayer (SLB) formation through variation in lipid concentration. **I. Alhallak**, P.J. Kett

CHED 1685. Development of a reusable colorimetric surface tethered polydiacetylene biosensor. **E.A. Pegues**, P.J. Kett

CHED 1686. Refinement of production grade biodiesel. K.C. McGill, **C. Axt**, **S. Ninneman**

CHED 1687. Thermal decomposition kinetics of select iodate salts. **M.H. Mellinger**, G.M. Bowers, R.K. Larsen

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CHED 1688. Equations for calculating limiting conductivities and ion-pair association constants for aqueous KCl under hydrothermal conditions. G.H. Zimmerman, **D.J. Staros**, H. Arcis, P.R. Tremaine

CHED 1689. Withdrawn

CHED 1690. Collisional energy transfer of highly vibrationally excited C_6H_6 at low temperatures. **J. Kuszynski**, N. West, J. Winner, Z. Buen, R. Bowersox, S.W. North

CHED 1691. Spectroscopic and computational study of metformin hydrochloride utilizing Raman under nitrogen spectroscopy to examine lattice structure. **T. Powell**, N. Hammer

CHED 1692. Study of the thermodynamics of fluoride-binding to understand the differences in the (heme pocket) structure and function of hemoglobin, myoglobin, and horseradish peroxidase. **A. Frankenfield**, D. Deysher, M. Lockwood, T.S. Nagle, K. Wodzanowski, J. Cerda

CHED 1693. Measurement of the activation parameters for fragmentation at penultimate proline in three tetrapeptides. **M.I. Dasch**, E.C. Sward, C.A. Gilmore, D.A. Hales, D. Fuller, T.J. El-Baba, D.E. Clemmer

CHED 1694. Reactivity of methane on Ni (111): Exploring high temperature surface sticking. **W. Coreas**, A. Mercier-Patterson

CHED 1695. Withdrawn

CHED 1696. Unusual structural features of halogen bonded and anion π complexes. **O. Grounds**, S.V. Rosokha

CHED 1697. Characterization of a covalently-linked dimer of rhodamine B using fluorescence correlation spectroscopy and fluorometry. **K. Griffith**, L. Pferdmenges, P. Lundin, K. Fogarty

CHED 1698. Synthesis of energy transfer systems utilizing guanosine and cytidine base pairing. **J. Hunter**, H. Owens, C.M. Lawrence

CHED 1699. Benzobisoxazoles cruciforms: Tunable, cross-conjugated platform for the generation of donor materials for organic solar cells. **L. Rainwater**, A. Burney-Allen, M. Jeffries-El, A.L. Tomlinson

CHED 1700. Silicate concentration effects in a "reverse chemical garden" reaction. **D. Chowdhry**, R. Palais, M.A. Horn

CHED 1701. Modelling the plant epicuticular layer with wax films. **S. Ly**, A. Edwards

CHED 1702. Organic crystals for THz generation. **L. Heki**, G. Valdivia-Berroeta, E. McMurray, S.J. Smith, D. Michaelis, J. Johnson

CHED 1703. Withdrawn

CHED 1704. Lifetime analysis of species in the laser-induced plasma using different energies on a variety of samples. **P. Morocho**, **A. Colon**, R. Chinni

CHED 1705. Molecular dynamics study of the photodissociation of ICN in ethanol. **A. Do**, N. Winter

CHED 1706. Gas phase structure and hydrogen/deuterium exchange of protonated tripeptides containing *L*-phenylalanine. **H.T. Vuong**, E.M. Marzluff

CHED 1707. Photoinitiated kinetics in a flow-tube: Characterization and first steps. **J. Scheeler**, A. Case, W. Merrill, F.F. Crim

CHED 1708. Temperature dependence of critical micelle concentration and of enthalpy of micelle dissolution for cetyltrimethylammonium bromide (CTAB) and dodecyltrimethylammonium bromide (DTAB). **H.E. Jackson**, L.C. O'Brien

CHED 1709. Development of an undergraduate-friendly single-molecule fluorescence system to study DNA base flipping and protein-DNA-interaction in UV-damaged DNA. **J.Y. Lo**, J.L. Godinez, C. Brummel, E.A. Aleman

CHED 1710. Withdrawn

CHED 1711. Photocatalytic study of the degradation of rhodamine B with reducible metal oxides. **R. Tritt**, A. Bhalkikar, A. Both, C. Cheung

CHED 1712. Kinetics of pseudo-first order phase transfer catalytic reactions. **X. Morrison-Wallace**, N. Shabestary

CHED 1713. Prebiotic potential of aerosols. **E. Shipley**, N. Bishop, J. Sebree

CHED 1714. Photophysical, electrochemical, and spectroelectrochemical characterization and solvent effect on the tautomerism of free-base corrole. **C.L. Reed**, **A. Leon**, **S.K. Mendez**, G.N. Calvillo, E.A. Aleman

CHED 1715. Decomposition pathways initiated by $Fe^+(^6D)$ and FeX^+ (X = Cl, Br, I) in halomethanes with significant global warming and ozone depleting potentials. **A.B. Eden**, C.L. Emmerling, W.S. Taylor

CHED 1716. RNA-based coacervate formation in the presence of macromolecular crowders. **B. Miller**, A. Marianelli, C.D. Keating

CHED 1717. Photoelectron spectroscopy experiments for the determination of electronic structure and reactivity of atmospheric ions: Ion trapping for improved temperature control. **K. Lister**, J. Melko

CHED 1718. Optimized photocatalytic synthesis of amides from amines and aldehydes. **K. Williams**, S.J. Gravelle

CHED 1719. Exploring the effects of differing concentrations of PTCDA on solar conversion efficiency and solar absorbance on TiO_2 catalyzed dye-sensitized solar cells. **H. LeClerc**, S.J. Gravelle, S.J. Pillsbury

CHED 1720. Characterization of a carbon dioxide-hexafluorobenzene complex using matrix isolation infrared spectroscopy. **Y. Payagala**, J.C. Amicangelo

CHED 1721. Fabrication and characterization of chalcone films with dispersed graphite nanoplatelets. **W. Bowling**, K. Cooper

CHED 1722. Investigating pharmaceutical crystal structures by ^{15}N chemical shift anisotropy. **J.T. Hosfelt**, S. Stuchell, R. Iuliucci

CHED 1723. *In situ* photo-kinetics and spectroscopy of organic aerosols. **N. Bishop**, E. Shipley, J. Sebree

CHED 1724. Binary phase diagrams of organic phase change materials. **D. Guo**, G.R. Van Hecke

CHED 1725. Structure of surfactant and polyelectrolyte stabilized hexadecane nanoemulsions. **B. Hickam**, A. Carpenter, G.L. Richmond

CHED 1726. Applications of TGA/DSC in energy science and energy geochemistry. **K. Huerta**, G.M. Bowers, S. Cunniff, R.K. Larsen

CHED 1727. Spectator ion effects in a "reverse chemical garden" reaction. **C. Cowley**, R. Palais, M.A. Horn

CHED 1728. Flow velocity effects in a "reverse chemical garden" reaction. **L. Butts**, R. Palais, M.A. Horn

CHED 1729. Characterization of the local dynamics of isotactic polystyrene in semi-dilute solution by NMR spin-lattice relaxation experiments and molecular dynamics simulations. **M. Meirow**, M.M. Fuson

CHED 1730. Laser ablation/molecular jet laser excitation spectroscopy of CaNCO. **D.M. Filion**, **B.T. Russ**, P.M. Sheridan

CHED 1731. Computational study of aluminum monoisocyanate isomers. **B.T. Russ**, P.M. Sheridan

CHED 1732. Raman spectroscopic studies of interactions between metal ions and ceramics. **K. Quist**, N. Hammer

CHED 1733. Characterization of DNA intercalation mechanisms of novel chemotherapy drug analogs. **K. Murphy**, **A. Peck**, S.S. Tartakoff, S. Glazier

CHED 1734. Raman spectroscopic and computational study of hydrogen bond interactions between urea, guanidine, and water. **A.D. Kamischke**, M.H. Byrd, S.A. Smith, D.H. Magers, N. Hammer

CHED 1735. Withdrawn

CHED 1736. Identification of unknown compounds produced in shock experiments. **J. Robbins**, V.P. McCaffrey, N. Zellner

CHED 1737. Analysis of commercial oxidative hair dyes using surface-enhanced Raman spectroscopy. **A. Henke**, N. Hammer

CHED 1738. Surface chemistry of crystal violet on titanium dioxide under acidic condition. **P. Raut**, K. Plotzke, J. Sebree, S. Coon

CHED 1739. Withdrawn

CHED 1740. Probing the structure and dynamics of the S21 pinholin protein. **R. Serafin**, D. Drew, G. Lorigan, I. Sahu, R. McCarrick, T. Ahammad

CHED 1741. Activation parameters for peptide cleavage at the penultimate residue: Dependence on identity of Yyy in XxxYyyGlyGly. **C.A. Gilmore**, M.I. Dasch, E.C. Sward, D.A. Hales, D. Fuller, T.J. El-Baba, D.E. Clemmer

CHED 1742. Raman under nitrogen spectroscopy (RUNS) and surface-enhanced Raman spectroscopy under nitrogen (SERSUN) of carbaceous materials. **C. Smith**, N. Hammer

CHED 1743. Studying the effects of hydrogen bonding in triazole and its derivatives. **L.A. Wallace**, A. Craig, J.H. Delcamp, G.S. Tschumper, N. Hammer

CHED 1744. Numerical and experimental study of calcium dynamics in the presence of environmental noise. **M. Moreno**, **C. Rosa**, S. Walker, J. Fry, S. Kadar

CHED 1745. Solubility, UV/Vis, and fluoresence study of various 2-aryl-3H-imidazo[4,5-b]pyridines. **A. Podgurski**, **S. Haddad**, K. Bernard, R.B. Mulligan, J.K. Murray

CHED 1746. Examining the photophysical properties of ibuprofen to develop a more effective method for screening drugs for photosensitive side effects. **N. Schug**, A. Bills

CHED 1747. Non-resonant two-photon excitation of photocaged compounds. **E. Lorenzo**, S. Senadheera, A.L. Houk, R.S. Givens, C.G. Elles

CHED 1748. Understanding the effect of osmotic pressure on the adsorption and rupture of phospholipid vesicles on a silicon dioxide surface. **A. Krone**, P.J. Kett

CHED 1749. Investigation of silica/titania composite materials doped with graphene oxide (GO) as substrates for plasmon-free surface enhanced Raman spectroscopy and analysis of GO defect density after thermal reduction. **L. Perez Morales**, E.J. Atkinson

CHED 1750. Effect of the Hofmeister series on supported lipid bilayer (SLB) formation. **I.H. Shah**, A. Krone, P.J. Kett

Section H
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Undergraduate Research Posters

Polymer Chemistry

Cosponsored by PMSE, POLY and SOCED
N. Di Fabio, J. Roberts, *Organizers*

12:00–2:00

CHED 1751. Developing and standardizing a methodology to investigate antibacterial surface coatings against *Escherichia coli* and *Staphylococcus aureus* . **R.T. Laemmle**, M. Jung, C. Horgan, A. Jaber, M. Yandian, E. Baulsir, R.W. Gurney, E. Scott

CHED 1752. Synthesis of an optoelectronic covalent organic framework from anthrone. **G.H. Pearson**, K. Allen

CHED 1753. Solid phase organic synthesis approach to polymers based on alternating ring opening metathesis polymerization. **I.H. Khan**, G. Li, G. Youn, L. Chen, N.S. Sampson

CHED 1754. Method for quantifying the oxidation within polymers using ATR-FTIR. **T. O'Keefe**, R. Duckworth, E. Hill, B. Hinderliter, M.A. Maurer-Jones

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CHED 1755. Quantification of environmental photo-crosslinking in poly(butylene adipate-co-terephthalate) polymer. **E. Monzo**, M.A. Maurer-Jones

CHED 1756. pH-responsive polymeric vesicles as drug delivery systems. **A.E. Dubos**, D. Fish

CHED 1757. Biomass based polyurethanes and the effects of stereochemistry on physical properties. **S. Silver**, J.G. Kennemur, R.J. Kieber

CHED 1758. Elaboration, characterization & biodegradation of partially bio-based polymer composites in aerobic and anaerobic conditions. **K. Wendover**, R. Bayard, V. Massardier, M. Valente, A. Quitadamo

CHED 1759. Modifying biopolymers for medically desirable outcomes. **A. Malik**, K. Broaders

CHED 1760. Polymers of intrinsic microporosity with photoswitchable azo functional groups. **J.H. Hsu**, M. Klemes, M. Haaf

CHED 1761. Surface initiated ATRP on SS316L for corrosion reduction. **E. Allego**, A.J. Rupprecht, A.M. Blystone, E.S. Gawalt

CHED 1762. Progress towards synthesis of an AB monomer for a Wittig polymerization. **H.J. Smith**, R. Posey, N.E. Huddleston

CHED 1763. Raster solvent vapor annealing of semi-crystalline homopolymer films. **D. Christiansen**, S. Bliesner, J. Albert

CHED 1764. Silyl ether-hydroxyl exchange in vitrimer systems. **H.J. Bates**, D.J. Fortman, W. Dichtel

CHED 1765. Aerosol preparation of spherical metal oxides for the purpose of surface modification. **A.L. Bielski**, F.C. Mayville

CHED 1766. Effect of molecular weight and acrylate ratio on glass transition temperature of ionomers. **D.M. Lewis**, K.A. Cavicchi, J. Marin Angel

CHED 1767. Calorimetry reveals differences in lipid membrane interactions of cell-penetrating peptides. **A. Folska**, L. Prevette

CHED 1768. Renewable polymers from itaconic acid. **A.R. Wong**, J.T. Trotta, A.M. LaPointe, B.P. Fors

CHED 1769. Synthesis of synthetic mimics enriched tryptophan copolymers for the use in antimicrobial studies. **J. Ewing**, S.G. Mankoci, A. Joy

CHED 1770. Exploration of drug release profiles of several NSAIDs encapsulated in varying chain lengths of polyethylene glycol (PEG) polymer-silica composites. **T.R. Kuntz**, D. Fish

CHED 1771. Acid-sensitive polymersomes from diblock copolymers for glucose-responsive insulin. **J. Queenan**, L.E. Prevette

CHED 1772. Characterization of polyhydroxyalkanoate enzymatic degradation products by mass spectrometry. **H.M. Blevins**, S. Baron

CHED 1773. Synthesis and characterization of porous starch-based adsorbents. **G.A. Lang**, **J. Castro**, I. Nelson, S.E. Naleway, C. Gorney, P.M. Iovine

CHED 1774. Polysaccharide-based hydrogels incorporating iodine-loaded starch granules. **M. Tran**, P.M. Iovine

CHED 1775. Synthetic routes to polyprene–polysaccharide conjugates via [4+2] cycloaddition intermediates. **B.J. Orzolek**, P.M. Iovine

CHED 1776. Probing the reactivity of amine-end functionalized starches. **J.B. Young**, C. Pham, P.M. Iovine

CHED 1777. Main-chain triazoline polymers and their conversion to poly(aziridines). **A.C. Saiz**, P.M. Iovine

CHED 1778. Indophenine as a donor-acceptor copolymer. **A. Helmin**, W.D. Wilcox, T.M. Pappenfus

CHED 1779. Tri-block copolymer self-assembles and biodegrades for drug delivery. **B.C. Haas**, L.E. Prevette, J.T. Ippoliti

CHED 1780. Acetylated and phosphoryl cholinated G5 poly(amidoamine) dendrimers for gene delivery: Balancing toxicity and DNA packaging efficiency. **T. Wieser**, L.E. Prevette

CHED 1781. Synthesis of G1-Ligand complex for nanotherapeutic drug delivery systems. **O. Morrison**, J.M. Manono, S.C. Dimaggio

CHED 1782. Investigating the binding thermodynamics of polycation-coated Au nanoparticles to gram-positive cell walls. **H. Ganzel**, L.E. Prevette

CHED 1783. Investigation of the antimicrobial activity of quaternized ammonium containing polymer chains. **C. Marick**, D. Fish

CHED 1784. Synthesis of monodisperse dendrimers for potential drug delivery materials. **B. Derbigny**, J. Manono, S.C. Dimaggio

CHED 1785. Analysis of intermolecular interactions in hydrazide containing metallogels. **Z.T. Armstrong**, J.L. Crane

CHED 1786. Preparation of surface-grafted poly(3-hexylthiophene) brushes using an easily cleavable self-assembled monolayer. **K. Campbell**, P. Lundin

CHED 1787. Synthesis of donor-acceptor dyads as a model for the active layer of single component organic photovoltaics. **R. Glass**, P. Lundin, G.B. Griffin

CHED 1788. Investigating novel hydrogel materials with thiol-ene click copolymerizations. **N. Schramm**, H. Zhu, J. Cubuk, M. Jani, D. Shah, S. Qavi, R. Foudazi, S. Rajaraman, P.G. Cohn

CHED 1789. Structure-property studies of anion-responsive liquid crystals. **H. Batchelor**, **B. Bouchard**, S. Cordero, L. Lam, K.A. Grabias, P.G. Cohn

CHED 1790. Improving the mechanical properties of Poly- β -valerolactone through aryl ring stacking and hydrogen bonding interactions. **F. Wenrich**, **L. Schroeder**

CHED 1791. Using multi-step synthesis for the production of hydrogels with adhesive properties. **M. Alcantar**, C.H. Lisse

CHED 1792. Investigating oxidized alginate-based fibers for biomedical applications. **A. Wilson**, W. Weeks, K. Penton, S.K. Hamilton

CHED 1793. Covalent organic frameworks for optoelectronic applications. **N. Sukanick**, K. Allen

CHED 1794. Synthesis of thermo-responsive functional poly(valerolactone) s via post-polymerization modification. **A. Yiu**, S. Sweningson, J. Hao

CHED 1795. Synthesis, self-assembly, and temperature-responsiveness of novel functional poly(valerolactone)s. **S. Sweningson**, A. Yiu, J. Hao

Implementing ACS Safety Education Guidelines
Sponsored by CHAS, Cosponsored by CCS and CHED

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

MONDAY EVENING

Section A
New Orleans Marriott Convention Center
Blaine Kern F

STRETCH Your Students' Minds by Using Materials to Engineer Ideas about Water, Food & Energy in the Chemistry Classroom

Financially supported by IPEC
S.C. Rukes, *Organizer, Presiding*

5:00 Introductory Remarks.

5:05 CHED 1796. Demonstrations and lab activities on a shoestring budget for all levels: A make and take session. **S.C. Rukes**

6:05 Intermission.

6:10 CHED 1797. Learning what AACT has to offer: Examples of resources from ACS and AACT. **J.L. Ball**, **S.C. Rukes**

6:45 CHED 1798. Ways of demonstrating and explaining matter and energy to middle school children. **J.D. Wilson**

7:20 Intermission.

7:25 CHED 1799. Converting chemistry activities to align with next generation standards. **K.B. Gosciniak**

8:00 CHED 1800. Augmented reality and the atomic model. **K. Cusachs**

8:35 Concluding Remarks.

Section B
ErnestN. Morial Convention Center
Halls D/E

Successful Student Chapters

N. Di Fabio, J. Roberts, *Organizers*

8:00–10:00

CHED 1801. Greening up the Reddies: Success with green chemistry at Henderson State University. **A. Eckerstorfer**, **C.M. Clem**, **C.W. Lechak**, **N. Steadman**, D. Bateman, B.A. Rowland

CHED 1802. Mississippi College's ACS student chapter: Using green chemistry in a garden. **K. Saleem**, **M. Martin**, T.D. Selby

CHED 1803. Motivating children, high school and undergraduate students with science through chemistry experiences. **A. Baez**, **D. Ciuro**, **K. Villa**, **A.S. Breton-Vega**, N.F. Morales-Penningston, J. Santos

CHED 1804. ACS-UPRB implementing community outreach through chemical education. **N.I. Estarellas San Miguel**, **D. Rivera-Rodriguez**, **R. Gracia Colon**, **C.D. Golderos-Trujillo**, **J. Ulloa**, L. Santiago, J. Oyola

CHED 1805. Fun of teaching teachers. **A. Guzman**, L. Santos

CHED 1806. Minot State University Student Chapter of the American Chemical Society. **J. Torgunrud**, M.M. Bobylev

CHED 1807. ACS Inter-Ponce food chemistry fun project. **S. Baez**, **C. Goicochea-Alvarado**, V. Torres Mejías, S. Meletiche Sepúlveda, A.G. Colon Santiago, E. Ferrer Torres

CHED 1808. Inter Ponce green division stands with Puerto Rico. **C. Cortes Bula**, **J. Costas Feliciano**, E. Ferrer Torres, A.G. Colon Santiago

CHED 1809. Friendship is magic: The Detroit Mercy Chem Club takes on sci-fi conventions. **M.J. Mio**, J. Pothoof, D.N. Maxwell, K. Suiter, R. Zouabi, T. Tieu Ngo, M. Bhagwagar, M.M. Payne

CHED 1810. Mole Day murder mystery: A chemical twist on a classic game. **M.J. Mio**, J. Pothoof, D.N. Maxwell, K. Suiter, R. Zouabi, T. Tieu Ngo, M. Bhagwagar, M.M. Payne

CHED 1811. Women in STEM: A topic worth discussion. **M.J. Mio**, J. Pothoof, D.N. Maxwell, K. Suiter, R. Zouabi, T. Tieu Ngo, M. Bhagwagar, M.M. Payne

Sci-Mix

C.V. Gauthier, A.L. Marsh, N.L. Snyder, *Organizers*

8:00–10:00

18, 58, 61, 88-89, 94, 105, 107, 109, 125, 127, 129-130, 131, 134, 136, 139, 146, 152, 170, 176-177, 179, 183, 191-192, 228, 231, 239, 243, 282-284, 1681. See previous listings.

1962, 1964, 1997, 2010, 2027, 2031, 2039, 2045, 2048, 2093, 2101-2102, 2106, 2129, 2133. See subsequent listings.

Section B
ErnestN. Morial Convention Center
Halls D/E

‡*Cooperative Cosponsorship*

CHED 1812. Academia Ponce Interamericana; promoting leadership and STEM. **A. Ruiz Ferrer**, **J.G. Noel Torres**, C.B. Pellicier Rodriguez, M. Negron Garcia, E. Ferrer Torres

CHED 1813. ACS Inter Ponce: Puerto Rico goes forward. **V. Torres Mejias**, **F. Rodriguez Reyes**, E. Ferrer Torres

CHED 1814. Making a difference: One group's work in community service. M. Nicolay, J. Bowlin, B. Graham, H.M. Payne, **M.W. Fultz**

CHED 1815. Understanding our Heritage: Learning the history of the Chemical Valley. J.P. Ricket, H. Aliff, **M.W. Fultz**

CHED 1816. Co-founders step-in to revamp the chemistry club after declining interest and participation. **M.M. Lopez**, N.A. Osti, Z. Barcenas, J. Salazar, M. Flores, M. Lopez, G.R. Shelton

CHED 1817. Inspiring tomorrow's society through the transforming power of chemistry. **L. Martir**, I. Montes, **G. Duran Camacho**, **D. Diaz**, **A. Rodriguez**, **S. Fuentes**, **J. Martinez**, **A. Gonzalez**, **E. Pagan**, **V. Soto**, **C. Maysonet**, **G. Colon**

CHED 1818. Mississippi College ACS student chapter activities and events. **J. Bethea**, **B. Montague**, **E. Robertson**, T.D. Selby

CHED 1819. Siena College Chemistry and Biochemistry Club: The benefit of being connected. **S.C. Curtsinger**, E.L. Smith, N. Howells, Z.T. Farina, J.L. O'Donnell, J.W. Karr

CHED 1820. ACS student member events, activities, and accomplishments at Duquesne University. E. Cooper, S. Shaik, L. Andreola, E. Castele, M. Baldwin, A. Schultz, P. Zakutansky, **H. Gering**, **E.R. Leung**, **K. McDougal**, **E. Allego**, **A. Miskalis**, P. Johnson, E.S. Gawalt, J.D. Evanseck

CHED 1821. Interrelationships between green chemistry, sustainability, and the community. X. Huang, C. Fisher, M.J. Kim, A. Klussmann, K. Johnson, A.M. Munro, **J. Freeman**

CHED 1822. Centenary College chemistry club: Connecting chemistry with community. **G. Doucet**, M. Abo-Zahrah, N. Walker, B. Jackson, T.M. Ticich

CHED 1823. Chapter activities for the Henderson State Univeristy Student Affiliate Chapter in 2017. **C.M. Clem**, **L. Russell**, **A.M. Noyes**, **C. Smith**, D. Bateman, B.A. Rowland

CHED 1824. Community engagement through chemistry and science education series. **C.M. Schreidah**, M.P. Klingberg, E.N. Kenney, G.T. Hymel, M.J. Demmings, E.T. Diemler, J.D. Koffman, O.M. Tharp, J.P. Fife, D.K. Kaeley, N. Mai, E.P. Kippenhan

CHED 1825. Infusing diversity and inclusion initiatives into the Student Chemists Association at The College of New Jersey. **S. Liang**, A. Smith, B.A. Bogin, C. Mileham, J. Steets, R. Goncalves, B.C. Chan, A.R. O'Connor, M.R. Bunagan

CHED 1826. South Dakota School of Mines and Technology: A successful student chapter of the American Chemical Society. **H.G. Leppert**, **J. Swanson**, K. Giorgio, **M. Acevedo**, J. Meyer

CHED 1827. Wayne State University American Chemical Society-Student Affiliates. **P. Marshall**, **D. Klemet**, **A. Prenkocevic**, **M. Silenski**, **A. Alnabolsi**, **R. Araj**, **M. Rayes**

CHED 1828. Delta State University ACS: Serving the MS delta through outreach and professional development. **A. Camarillo**, Z.K. Kinler, K. Penton, S.K. Hamilton

CHED 1829. Dynamic activities of the ACS student chapter at Inter American University of Puerto Rico -Metropolitan Campus. K.A. Parga Rivera, **P.E. Peña-González**, **K.F. Coballes**

CHED 1830. Fund raising as a compromise to maintain the student chapter united. **G.E. Martínez Bracero**, E.d. Franceschini Silva, S.M. Vargas Padilla, E.N. Garcia Acosta, P.N. Silvestry Padilla, A. González Mederos

CHED 1831. Withdrawn

CHED 1832. Successful ACS student chapter at Wilkes University: Community outreach events that apply green chemistry principles and science education. **A. Black**, N. Fitzpatrick, J. Larsen, H. Arcure, M. Youmans, C. Henkels

CHED 1833. Chemistry is central at UCO. **C.B. Frech**, D.R. Rundle, G. Rodriguez, E. Cline, K. Bennett, E. Welander, L. Brown, M. Raischel

CHED 1834. Grizzlies get their growl on: Georgia Gwinnett College chemistry outreach. **A. Ko**, **M. Roark**, **K. Coscia**, **D. Munna**, R.K. Kalman, G.E. Rudd

CHED 1835. Saint Francis University Chemistry Club: Creating unbreakable bonds. **P.T. Kasunic**, **M.E. Hogue**, K.S. Patterson, H. Schorr, E.P. Zovinka

CHED 1836. IVCC finds the perfect solution. **R. Schulz**, J. Hall, M.E. Johll, P.K. Yong

CHED 1837. KU Chemistry Club: Strength through recruitment, engagement, and professional development. **E. Lorenzo**, C.D. Clay, R.M. Walsh, K. Kao, R.S. Black

CHED 1838. Activites of the Southwestern Oklahoma State University Chemistry Club. **W. Hill**, **E. Allbritton**, **E. Hicks**, **D. Widick**, **K. Shoff**, J.C. Henrikson, T.K. Ellis, L. Gwyn

CHED 1839. Student Members of the American Chemical Society, Hofstra Chapter. **A. Sica**, G. Kroening, H. Tarbox, M. Saleem, M. Currie, V. Zhang

CHED 1840. Creating a community at Stony Brook University. **C. Weidner**, J.A. Daly, K. Nickson, J.E. Zambito, J. Mallon, J. Zheng, K. Aubrecht

CHED 1841. Chemistry Rocks at Georgia College. **M. Schellman**, A. Hanna, E. Bullington, A. Stapleton, T. Oderinde, C.H. Lisse

CHED 1842. Urban vegetable garden: Study of nutrients and limiting factors in plant viability. **J. Daye**, **L. Valientes**, N. Fernandez, A. Vega, T.L. Hall, K. Pierre, M. Lewis

CHED 1843. Erskine Chapter ACS: A catalyst in our community. **K. Squiggins**, K. Richey, A.C. Hartley, P.A. Skerratt, A. Coker, J.E. Boyd, T.R. Hayden

CHED 1844. Chemistry, community, camaraderie, and career preparation: Realizing the "Four C's" through student activities at the University of New England. **K.A. Chalmers**, **J. White**, A.E. Keirstead

CHED 1845. Chemistry Fun at NSU. **A. Chung**, **S.B. Vazquez**, B. Aukszi, M. Ballester

CHED 1846. TCU Chemistry Club: Community STEM educations programs in DFW and methods of organization and communication. A. Vu, M.M. Barnett, B. Niebuhr, N. Schmitt, T.M. Schwartz, K. Ji, K. Wegener, K. Chaker, C. Keller, J. Snowden, H. Conrad, J. Fry, **K.N. Green**

CHED 1847. Spreading interest and opportunities in chemistry from elementary schools to universities in Philadelphia. **J. Olivencia**, K. Strouse, S.A. Fleming

CHED 1848. American Chemical Society Student Chapter of Idaho State University. **B. Poulter**, M. Mangun, S.F. Spradlin, L.J. Maxton, E.A. Morley, J.J. Pak, C.M. Evilia

CHED 1849. Santa Monica College Chemistry Club promotes community involvement and environmental awareness. **D. Sulca**, **K. Wannemo**, **T. Meziab**, **A. Gaynes**, **C. Lee**, **A. Ignant**, T. Pecorelli, J.M. Hsieh

CHED 1850. DeSales University Student Affiliate of ACS. **B. Gillott**, **K. Alderfer**

CHED 1851. SIUE Chemistry Club: Promoting chemistry and science learning to the campus and community abroad. **H.K. Lupton**, G. Hansen, S. Hayes, R. Bryant

CHED 1852. Kent State SAACS: Rebuilding a Chapter. **S. Kempf**, Y. Zheng

CHED 1853. Green chemistry and outstanding chapter award winning activities of Midland College Chemistry Club. **D. Bloomgren**, **S. Mohiuddin**, **N. Adams**, **Z. Isa**, **M. Martinez**, **J. Anderson**, **P. Kesavan**

CHED 1854. Mad Scientist Day junior event impact on Birmingham, Alabama. **R.J. Murphy**, **E. Quarato**, **K.C. Deneen**, J.A. Nikles

CHED 1855. Developing into a outstanding student chapter: A student focued approach. **D. Gepford**, **T. Ostrom**, **A. Stothard**, J.M. Groenevelt, R. Adams, D.J. Lecaptain

CHED 1856. UCA ACS: Power in numbers. **S. Margis**, **S. Turner**, **C.L. Emmerling**, **E.N. Tran**, **J. Schneider**, **S. Stokes**, G.R. Naumiec, F.M. Yarberry

CHED 1857. Straight out of Compton... Science Center. **A. Jones**, **S. Marcelino**, B.N. Norris

CHED 1858. Activities of the Spelman College ACS Chapter. **K. Fontan**, F. Fullilove

CHED 1859. Park University CHEM Club 2017-2018. **J. Pham**, G. Stelmacovich, A. McMullen, J. Berry, M. Klein

CHED 1860. Increasing chemistry outreach in Southeast Missouri. **K. Ihns**, **H. Hufford**, **K. Jefferson**, **H. Hufstedler**, **K. Bunselmeyer**, **B. Miller**, S.E. Shaner, C. Ragain

CHED 1861. Catawba College shows chemistry rocks. **T.D. Williams**, C. Saner

CHED 1862. Chemistry in Boston: Northeastern University Student Chapter bonding with its communities. **D. Dang**, J.Y. Chen, S. Narasimhan, D. Cehreli, L. Po

CHED 1863. Otterbein Student Chapter: Moving involvement off campus. **E. Isaac**, D.H. Johnston

CHED 1864. Serving with science: Outreach with the UM-Flint Chem Club. **C. Wilhelm**, **D. Corey**, **L. Harris**, **N.D. Alawwa**, **M. James**, **E. Kiser**, **M.K. Alsarraj**, M.R. Wilhelm, J.L. Tischler

CHED 1865. Millersville University American Chemical Society Student Chapter. **J.E. Thames**, S.K. Gillis, G.H. Pearson, L. Ostopowicz

CHED 1866. Tarleton Chemical Society–sharing our past, celebrating our future. **K.L. Bullard**, **J.D. Murphy**, L.D. Schultz

CHED 1867. Olivet College Gruen Chemistry Society: Student affiliate activities. **B. Sturgeon**, **J. Kiess**, **A. Gruszka**, **I. York**, S.M. Lewis

CHED 1868. Science club activities at the College of Mount Saint Vincent for 2017-2018. **T. Chin**, **N. DeSouza**, P.K. Kerrigan

CHED 1869. Southeastern Oklahoma State University ACS Student Members: 50 years of chemistry from the savage storm. **E. Landers**, **P.S. Whitehead**, **S. Goff**, **A. Castaneda**, **P. Thomas**, **N.L. Paiva**

CHED 1870. Saint Vincent College Chemistry Club. **J.A. Hungerford**, K.A. Thomas, H.N. Hosack, J. Centore, D. Fish

CHED 1871. Xavier University of Louisiana's ACS Student Chapter: A chemical force for good in the greater New Orleans area. **J. Adkins**, **A. Andre**, **R. Miles**, **J. Malone**, **E. Cubit**, **M. Crawford**, **A. Stephens**, **A. Madison**, M.R. Adams, C.M. Lawrence

CHED 1872. Promoting chapter growth within Nittany Chemical Society with increased collaboration and events. **E. Gogarnoiu**, L.C. Velazquez Bello

CHED 1873. Balancing the right campus involvement equation. **S.M. Szwedo**, J. Desai, I.D. Lykens

CHED 1874. Barry University Chemistry Club: Fostering an inclusive scientific sommunity and improving science outreach every day! **L. Mesa**, E. Paulus, D. Cordero, N.A. Maxi, C. Joseph, **G.H. Fisher**, T. Hamilton

CHED 1875. ACS UPR-Aguadilla an outstanding legacy: 15 years of successful history. **C.M. López-Hernández**, **M.L. González-López**, **S.M. Escobar Avilés**, R.A. Estremera-Andújar, C.A. Nieves-Marrero, B.J. Ramos-Santana

CHED 1876. SMSU Chemistry Club through the years. N.J. Beyer, **V.J. Henry**, **E.J. Popma**

‡*Cooperative Cosponsorship*

CHED 1877. Aquinas Chemistry Society: Service, leadership and education. **N. Strobel**, **M.P. Mata**, **A. Gaspar**, **S. Clark**, **S. Hicks**, E.A. Jensen

CHED 1878. Creative uses of National Chemistry Week themes throughout the years by Florida International University, Biscayne Bay Campus Science Club. **D. Read**, J. Glenny, **S. Castaneda**, M. Michel, M. Wharton, **M. Delgado**, L. Valientes

CHED 1879. Pasadena City College (PCC) Chemistry Club. **F. Castro**, **J. Hernandez**, **V.I. Jaramillo**

CHED 1880. Molloy Chemical Society. **L. Bui**, **E. Brutschea**, **I. Armento**, A. Russell

CHED 1881. Fat Tuesday: Nexus of food, energy, and water. **L. Farber**, S.W. Baer, R. Russo, C. Domville, H. Jia, B. Kalach, R. Yozzo, A. Balesano, B. Yesko

CHED 1882. Take it to the hood: Effective ways to engage the campus and surrounding community. **J. Gearhart**, C. Kristoff, A. Freiberger, J. Layton, C. Gething, E.A. Baldauff

CHED 1883. Suffolk University: Outreach, involvement, education. **K. Jenkins**, L. Huoth, B. Gemechu, L. Riffert, N. Grimaud, E.J. Enyedy

CHED 1884. On the road again: Developing our chapter through service, locally and beyond. **L. Atlas**, Q. Dougherty, V. Ganss, A.H. Kjellson, S. Lareau, I.J. Levy

CHED 1885. ACS Student Chapter at the University of Utah. A.D. Loret, S. Lee, M. Pham, R. Reynolds, A.M. DeGrauw, D. Drapeau, S. Morgan, **C. Coplan**, K. Alvarez, A. Thomas, A. Borodai, H.L. Sebahar, T.G. Richmond

CHED 1886. ACS student chapter at the University of Tennessee at Martin. **S.E. Max**, S. Oliva, T. Rinehart, B. Ide, A.H. Shelton

CHED 1887. Catalyst for a brighter future: UCSD American Chemical Society-Student Affiliates. **S. Lee**, T.J. Bussey

CHED 1888. Chemistry Club at Carthage College. **B. Bresnahan**, L. Sanford, R. Geoghegan, H. Miles, L. Hall, S. Franklin, J.S. Kirk

CHED 1889. Eastern Oregon University ACS Student Member Chapter: Promoting community outreach and professional networking. **Q.C. Durfee**, J.D. Jacobs, M. Wynn, E.J. Holeman, B.L. Stavaas, A.G. Cavinato

CHED 1890. American Chemical Society Student Chapter at the University of St. Thomas, Houston, TX. **A.V. Hernandez**, **C. Luong**, **Y. Tran**, V. Hoang, A. Nguyen, E. Evans, C.A. Young, J. Hollingsworth

CHED 1891. Lobo Chemistry Club: American Chemical Society student chapter at the University of New Mexico. **E. Hjelvik**, **C. Hunter**, **B. Villalva**, **K. Thompson**, **J.R. Terr**

CHED 1892. Inspiring scientists of the future: Encouraging diversity in the STEM fields. **M.E. Hackey**, K. Letson, H. Wakidi, S.K. O'Shea, C. Murphy

CHED 1893. Chemistry outreach with Heidelberg University's ACS Chapter. **K. Scrudders**, A.F. Bauer, D. Blum, R. Webb, R. Raimondo, N. Beres

CHED 1894. Student members of the American Chemical Society at the University of Tampa. **N. Zembol**, **L. Truesdale**, J.A. Struss, L. Henchey

CHED 1895. University of Minnesota-Morris ACS student chapter. **D. Schultz**, E. Trieu

CHED 1896. Western Washington University Student Chapter of the American Chemical Society. **C. Crickmore**, S. Neely, **S.R. Emory**, E. Raymond

CHED 1897. Highlights of the activities of the University of Szeged ACS Student Chapter. **B. Bohner**, B. Csipak

CHED 1898. Making the connection between science and crime solving with today's youth. **J. Stetzler**, A. Colon

CHED 1899. Teaching and engaging students toward the use of green chemistry approaches. **G. Uzcategui-White**

CHED 1900. Carroll University Chemistry Club. **R. Kutzner**, **A. Tomczyk**, **D. Daujatas**, **K. Burke**, N. Popp, A. Larsen, V. Wagner, K.E. Molter

CHED 1901. Missouri Western State University Alchemist Club: Making science great (again). **C. Watson**, **R. Prest**, **M. Phillips**, J. Moore, J.E. Wagner, D. Stasko

CHED 1902. Tiffin University: Building a Successful Chapter. **T.N. Lewis**, **A. Flotteron**, **B. Utley**, **S. Hitchcock**, M. Sabo

CHED 1903. Leading a successful ACS student chapter. **L.M. Louis**, S. Botha, D. Brenning, R. Wooten-Moyer, A.J. Sanders

CHED 1904. Chemistry and community: ACS at Ouachita Baptist University. **A. Cole**, **J. Cook**, J.E. Bradshaw, S.E. Hubbard

CHED 1905. Student chapter events and activities done at Tennessee Tech University. M. Dunn, **W. Parker**, T. Pinto, K. Lawson, S. Jones, R. Baker, K. Lyons, J. Scantland, J.G. Coonce, A.J. Carroll

CHED 1906. Bolstering Campus-wide undergraduate interest in chemistry with a "MinesCraft" themed research fair. **D. Isaak**, **J.C. Larrabee**, A. Biery, A.G. Caster

CHED 1907. Creating an engaging ACS chapter at a private university. **C. Azaldegui**, J. Belmares, D. Ivan, L.A. Mayorga, D. Saldana, M. Kopecki Fjetland

CHED 1908. Loras College American Chemical Society Accredited Club. **L. Schroeder**, **S. Neuzil**, **A. Miller**, **A. Carter**, **D. Dahlberg**, **S.E. Hammer**, D.J. Oostendorp

CHED 1909. UT Tyler ACS Student Chapter. **C. Hjorth**, **J. King**, L.A. Johnson, L.E. Boyd

CHED 1910. Forensic chemistry division: Guiding for a safe society. **J. Negron Rodriguez**, **C. Cabrera Lopez**, E. Ferrer Torres

CHED 1911. Morehead State University Chapter of the American Chemical Society. **C. Sullivan**, **S. Little**, M.T. Blankenbuehler

CHED 1912. ChEmory: Emory University's undergraduate chapter of the American Chemical Society. **D.C. Salgueiro**, A. Diaz, A. Syed, D.R. Mulford, J. Omar, S. Hwang, J. Narula, T. Kowal-Safron

CHED 1913. Building a Successful ACS Student Affiliate through professional development, community outreach & community service. S. Cunningham, R. Mcfarland, C. Gunnell, **R.V. Valcarce**, P.J. Iles, L.D. Giddings, N.R. Bastian, W.C. Sanders, M. Alvarez

CHED 1914. Chemistry Rocks – Wesley College's 2017 afternoon of fun. **A. Jean-Francois**, M.J. D'Souza

CHED 1915. Florida Southern College ACS student chapter growth 2017-2018. **J. Marshall**, A. Branch, K. Martinet, K. Alexander, I. Mauzy, B. Tyson, J.F. Eubank

CHED 1916. Fostering professional development and inter-chapter relations through the Annual Florida Chemistry Conclave. **J. Kreisel**, **S.M. Kuebler**, L. Gandy, **R. Sapia**, N. Takenaka

CHED 1917. SAACS: Year one in review. **C. Beeler**, S. Barnett, M. Beeler, W. Bowling, S. Greer, C.J. Leatherwood, Z. Neverstitch, A.L. Thomas

CHED 1918. Lock Haven University Chemistry Club. **S. Shreiber**, S.J. Sujansky, T.J. Adams, K. Range, K.T. Root

CHED 1919. Ball State University Student Affiliates of the ACS: Science for everyone. A. Waggoner, B. Watson, **S. Pruitt**, **L. Milton**, **C. Barrios**, D. Dooley, R. Jeske

CHED 1920. Inspiring passion and educating others through chemistry and biochemistry. **A. Pagano**, **J. Maung**, **L. O'Connor**, **R.A. Riley**, M.G. Paulick

CHED 1921. Colorado State University Chemistry Club: Engaging the community through science. **N. Knostman**, J.T. Brookhart, C. Henderson, L.N. Paricio, A. Rauker, I. Sitarik, J. Trowbridge, B.P. Reynolds

CHED 1922. Stanislaus State Warriors Chemistry Club: Connecting and sharing with the community. **J.Y. Lo**, **J.A. Garfield**, C.L. Reed, J.L. Godinez, A. Leon, P. Ayson, E.A. Aleman

TUESDAY MORNING

Section A
New Orleans Marriott Convention Center
Blaine Kern C

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Cosponsored by ANYL‡, COLL‡, ENVR‡, INOR, PMSE‡ and PRES‡
B. Barnes, S. Locicero, B. Olson, N. Richey, Y. Zhang, *Organizers, Presiding*
M. Sims, *Presiding*

8:45 Introductory Remarks.

9:00 CHED 1923. Exploring the ultimate limits of miniaturization. **P.S. Weiss**

9:45 CHED 1924. Synthesizing molecules by atom manipulation – an atomic scale look at molecular transformations. **B. Schuler**, N. Pavliček, N. Moll, G. Meyer, L. Gross

10:15 Intermission.

10:30 CHED 1925. Designing nanoparticles for sustainability. **C.L. Haynes**

11:00 CHED 1926. Surface chemistry controlled optoelectronics of small metal nanoparticles. **J. Millstone**

11:30 CHED 1927. Sunlight-driven hydrogen formation by membrane-supported photoelectrochemical water splitting. **N.S. Lewis**

Section B
New Orleans Marriott Convention Center
Blaine Kern A

George C. Pimentel Award in Chemical Education

Cosponsored by WCC
D.M. Bunce, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED 1928. Support by the National Science Foundation for the development of peer-led team learning. **S.H. Hixson**

9:00 CHED 1929. PLTL: A multidisciplinary intervention to ensure success in STEM gatekeeper courses at morehouse college. **L.S. Young**

9:20 CHED 1930. Three Big P's: POGIL, PLTL, and Pratibha. **R.S. Moog**

9:40 CHED 1931. Oh, the places you'll go: The dissemination and implementation of the peer led team learning project, a unique student-faculty partnership. **I. Druwe**

10:00 CHED 1932. Implementation and evolution of PLTL in introductory computer science courses. **S. Rodger**

10:20 Intermission.

10:30 CHED 1933. Peer led team learning applied to laboratory instruction. **J.P. Dinnocenzo**

10:50 CHED 1934. PLTL: Experience from both sides of the desk. **J. Kinsella**

11:10 CHED 1935. From face-to-face to online: Collaboration in design and implementation of cPLTL. **K. Mauser**, **J. Sours**, L. Zhu, P. Varma-Nelson

11:30 CHED 1936. Peer-led team learning in science and engineering at IUPUI. **S.J. Rhodes**, E. Adams, S. James, C. Krull, S. Lauhlé, D. Malik, R.E. Minto, S. Mukhopadhyay

11:50 Concluding Remarks.

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Active Learning in the General Chemistry Curriculum

J.K. Robinson, *Organizer*
R.M. Henry, *Presiding*

8:30 CHED 1937. Case study of case studies: Writing choose-your-own-experiment cases and avoiding common

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pitfalls that decrease case study use. **J.K. Hines**

8:50 CHED 1938. Active learning with clickers and small groups in general chemistry. **D.J. Weiss**, P. McGuire

9:10 CHED 1939. Overcoming barriers and obstacles to casually implement student-centered active learning activities incoporating computer simulations in a large lecture setting for students enrolled in a general chemistry course sequence. **T.J. Greenbowe**, D.B. Exton, J.I. Gelder, M.R. Abraham, D.R. Sullivan

9:30 CHED 1940. Bridging the gap: Enhancing engagement in a large gen chem class with differentiated activities & formative assessment. **A.G. Caster**, R.L. Falconer, A. Sower

9:50 Intermission.

10:05 CHED 1941. A progression of active learning integration in general chemistry courses. **K.J. Linenberger Cortes**, M.L. Head

10:25 CHED 1942. Overcoming student resistance to active learning through interventions that advocate a growth mindset. **T.D. Shepherd**

10:45 CHED 1943. Active learning in large general chemistry classes through flipped peer led team learning: Implementation and evaluation. **S.E. Lewis**, J. Robert

11:05 CHED 1944. Flipped Fridays in a large general chemistry course. **D. Meyer**

Section D
New Orleans Marriott Convention Center
Blaine Kern B

Green Chemistry Theory & Practice: Food, Energy & Water Sustainability

Cosponsored by CEI
Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision

E.J. Brush, *Organizer*
J.E. Wissinger, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 1945. The green chemistry commitment: Progress and future plans. **A.S. Cannon**, D. Ward

8:55 CHED 1946. Developing a multidisciplinary bachelor of science degree in green chemistry at the University of Michigan-Flint. **N.B. Kingsley**, **J.L. Tischler**

9:15 CHED 1947. Painting more homes green in the chemistry curriculum. **E.A. Jarvis**

9:35 Intermission.

9:50 CHED 1948. Green chemistry education roadmap: Systems thinking in the chemistry curriculum. **J. MacKellar**

10:10 CHED 1949. Research experience for undergraduates: Food, energy and water security at Mississippi State University. D. Mlsna, **T. Mlsna**

10:30 CHED 1950. Development of a green chemistry protocol for planning and conducting undergraduate research. **K.M. Halligan**

10:50 CHED 1951. Using place to integrate environmental justice, sustainability and green chemistry into the curriculum. **L. Bastin**

11:10 CHED 1952. Exploring connections between green chemistry, equity, and environmental justice. **E.J. Brush**

11:30 Discussion.

Section E
New Orleans Marriott Convention Center
Fulton

Research in Chemistry Education

M. Anzovino, J.H. Carmel, *Organizers*
J. Harshman, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 1953. Utilization of a modified gradual release of responsibility model in a large enrollment chemistry course. **N. Lapeyrouse**, C. Yestrebsky

8:55 CHED 1954. Peer-supported learning in undergraduate chemistry: A comparison of learning assistants and a tutoring center. **R.M. Jones**

9:15 CHED 1955. Investigating the impact of using transformed curriculum materials on structure-property relationships in a traditional general chemistry course. **A.T. Kararo**, G. Gadi, S.M. Underwood

9:35 CHED 1956. High school science teachers' understandings of the practices of science and engineering. **M. Orgill**, J. Adams, S. Nealy, C. Kardash

9:55 Intermission.

10:30 CHED 1957. Characterization of complexity of general chemistry students' reasoning in argumentative writing about ocean acidification. **A.C. Moon**, R. Moeller, A. Gere, G.V. Szymczak

10:50 CHED 1958. Investigating the impact of an alternative general chemistry curriculum among diverse classroom environments. **S.M. Underwood**, A. Pollock, M. Cooper

11:10 Concluding Remarks.

Section F
New Orleans Marriott Convention Center
Blaine Kern E

Chemistry Learning & Math Learning: Which is the Cart & Which is the Horse?

M.H. Towns, *Organizer*
K. Bain, *Organizer, Presiding*

8:30 CHED 1959. The structure of mathematical reasoning with proportions and implications for chemistry teaching. **D.J. Wink**

8:50 CHED 1960. Rigor in general chemistry doesn't equal math: The role of systems thinking. **T. Holme**

9:10 CHED 1961. Chemistry problem solving: an investigation of mathematical reasoning skills. **D.A. Canelas**, B. Cooke

9:30 CHED 1962. Characterizing cognitive processes involved in chemical kinetics: Using a blended processing framework to describe students' chemistry and mathematics knowledge interactions. **K. Bain**, J.G. Rodriguez, A. Moon, M.H. Towns

9:50 CHED 1963. Exploring the interrelations between affective and cognitive dimensions of mathematics and chemistry learning. **M. Mack**, L. Goldman, C. Stanich, S. Freeman

10:10 Intermission.

10:25 CHED 1964. Helping students transfer math knowledge into general chemistry using online, adaptive modules. **C. Richardson**

10:45 CHED 1965. Early mathamatics intervention to improve success in survey chemistry courses. **M.J. Castaldi**, **B. Monari**, M.A. Bailey, B. Gallager, P. Jameson, J.K. Murray

11:05 CHED 1966. Trying to predict success in general chemistry: Lessons learned from a systematic study of our admissions data. **J.R. Williams**

11:25 CHED 1967. Influence of chemistry and mathematics placement exam scores on PLTL success. **D. Malik**, L. Zhu, M. Nguyen

11:45 CHED 1968. Math and chemistry research as tools to encourage and foster urban high school students in STEM fields. **B. Kunnath**, G. Bonomo, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

12:05 CHED 1969. Learning to read spectra: Teaching deconvolution with Excel in a Scientific Writing course. **R. Glaser**, A. Muelleman

Section G
New Orleans Marriott Convention Center
Magnolia

Advancing Undergraduate Research in Chemistry: Best Practices & New Innovations

Early Course Integration

R.M. Jones, *Organizer*
B.L. Gourley, *Organizer, Presiding*
A.G. Cavinato, *Presiding*

8:30 Introductory Remarks.

8:40 CHED 1970. A redesign of the first general chemistry lab session: Introducing the research process. **D.A. King**, **B.B. Magers**, P.L. Stan

9:00 CHED 1971. Implementation of a course-based crystallography research project in the general chemistry laboratory. **R. Morgan Theall**, **S.E. Shaner**, **M. Bond**

9:20 CHED 1972. First year undergraduate research experience. **J. Wallach**

9:40 CHED 1973. Engaging early-career undergraduate students in research enhances the Gustavus Adolphus College chemistry program. **B. Russell**, **S. Bur**

10:00 Intermission.

10:10 CHED 1974. Green organic chemistry research with undergraduate students. **M. Hunsen**

10:30 CHED 1975. CRSP: Formalizing undergraduate research at Kingsborough Community College. **H.S. Barcena**, D. Berhanu

10:50 CHED 1976. An undergraduate peer-mentoring research model as a for-credit course during the academic year. **S.G. Tajc**

11:10 CHED 1977. Development of an undergraduate research methods course to satisfy the ACS CPT guidelines and the Quality Enhancement Plan at Tennessee Technological University. **A.J. Carroll**, M.N. Halwani

Chemical Information Literacy: Innovation, Collaboration & Assessment
Sponsored by CINF, Cosponsored by CHED

Undergraduate Research in Polymer Science
Sponsored by POLY, Cosponsored by CHED and PMSE

TUESDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
Blaine Kern C

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Cosponsored by ANYL‡, COLL‡, INOR, PHYS‡, PMSE‡ and PRES‡
B. Barnes, S. Locicero, B. Olson, N. Richey, M. Sims, Y. Zhang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 1978. Evolutionary and concurrent design of photonic nanostructures. **T.W. Odom**

2:05 CHED 1979. Nanoscale engineering of efficient oxygen reduction electrocatalysts by tailoring the local chemical environment of Pt surface sites. **S. Linic**

2:35 CHED 1980. There's even room to expand at the bottom: A story of "giant" nanocrystals. **J.A. Hollingsworth**

3:05 Intermission.

3:20 CHED 1981. Polymerizations with elemental sulfur: Making weird polymers in weird times. **J. Pyun**

3:50 CHED 1982. Metallo-supramolecular polymers: From stimuli-responsive materials to poly[n]catenanes. **S.J. Rowan**

4:20 CHED 1983. The art of building small, from molecular switches to motors. **B. Feringa**

4:50 Concluding Remarks.

Section B
New Orleans Marriott Convention Center
Blaine Kern A

George C. Pimentel Award in Chemical Education

Cosponsored by WCC
D.M. Bunce, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 CHED 1984. Theoretical cognitive foundations for peer-led team learning.

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M.S. Cracolice

2:00 CHED 1985. Assessing the development of curved-arrow formalism mastery among first-semester organic chemistry PLTL and cPLTL students. **S.B. Wilson**, P. Varma-Nelson

2:20 CHED 1986. Peer-led team learning and Pratibha Varma-Nelson – irrepressible and resilient. **J.E. Lewis**

2:40 CHED 1987. Attending to the subject. **B.P. Coppola**, J.R. Boothe, R. Barnard, L.J. Peterson

3:00 Intermission.

3:10 CHED 1988. Transferrable skills gained from experience as a peer-leader in a PLTL program: Reflections, applications, and long-term impacts on professional lives. **A. Chase**, A.S. Rao, P. Lakamala, P. Varma-Nelson

3:30 CHED 1989. Course-based undergraduate research via the CASPiE project: From idea inception to cross-institutional networks. **G.C. Weaver**

3:50 CHED 1990. Bringing peer learning into the laboratory and research setting. **D.J. Wink**

4:10 CHED 1991. Award Address (George C. Pimentel Award in Chemical Education Sponsored by Cengage Learning and the ACS Division of Chemical Education). Reflections on a non-traditional academic career: Lessons for the future. **P. Varma-Nelson**

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Active Learning in the General Chemistry Curriculum

J.K. Robinson, *Organizer, Presiding*

1:30 CHED 1992. Modified, clicker-based peer-Instruction in an active, flipped classroom. **D.M. McGregor**, M.A. Deri, P. Mills

1:50 CHED 1993. Active learning in large courses: Challenges and solutions. **R.D. Link**

2:10 CHED 1994. Active learning in general chemistry at Marquette: From flipped to studio courses. **S.A. Reid**, M.D. Ryan, A.T. Fiedler

2:30 CHED 1995. Engaging participation and promoting active learning through student usage of the internet to create notes for general chemistry in class. **R.M. Henry**

2:50 Intermission.

3:05 CHED 1996. Implementing retrieval practice with Moodle to enhance student learning in chemistry. **G. Lo**

3:25 CHED 1997. Analysis of active learning recitation program for Chemistry I at Mississippi State University. **V.L. Perera**, D. Mlsna

3:45 CHED 1998. Breaking the mold of a "weed out" course: The development of an applying critical thinking in various elements (ACTIVE) learning program to help struggling students with deficiencies in prerequisite STEM education. **C. Kelleher**, B. Turnpenny, A.S. Silva

4:05 CHED 1999. Flipped classrooms, peer assistants, and tutoring: The winning combination at USM. **L. Benedict**, P. Dexter

Section D
New Orleans Marriott Convention Center
Blaine Kern B

Green Chemistry Theory & Practice: Food, Energy & Water Sustainability

Cosponsored by CEI
Financially supported by ACS Green Chemistry Institute; I&EC Green Chemistry Subdivision
J.E. Wissinger, *Organizer*
E.J. Brush, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 2000. Green context-based electrochemistry lab for general chemistry. **S. Couture**, N. Abd El Meseh, H. Sevian

1:55 CHED 2001. Investigation of phenylsemicarbazone and phenylthiosemicarbazone synthesis in green solvent systems. **W. Evans**, J. Bennett

2:15 CHED 2002. Life cycle inventory assessment as a sustainable chemistry and engineering education tool. **M. Sabahi**, E. Reichmanis

2:35 Intermission.

2:50 CHED 2003. Green chemistry as a theme: Development of green inquiry labs and students impressions. **D.C. Bromfield-Lee**

3:10 CHED 2004. Definition and evaluation of sustainability indicators for biodiesel production. **V. Gude**, E. Martinez-Guerra

3:30 CHED 2005. Starting with vanillin: Two-step synthetic sequence illustrating green chemistry principles. **J.E. Wissinger**, J. Palesch, B.C. Gilles

3:50 Intermission.

4:05 CHED 2006. Green chemistry: Preparing students to meet the grand challenges of sustainability. **K. Aubrecht**, **M. Bourgeois**, **E.J. Brush**, **J. MacKellar**, **J.E. Wissinger**

4:25 Panel Discussion.

Section E
New Orleans Marriott Convention Center
Fulton

General Papers

S.A. Fleming, *Organizer*
R. Broyer, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 2007. Using cognitive load theory (CLT) based problem sets to improve problem solving skills in general chemistry courses. **D. Behmke**, T. Gluick, B. Shepler, J. Sloop, C. Woodbridge, J. Mielke

1:55 CHED 2008. Development of a concept inventory to bridge the gap between general and organic chemistry. **R. Broyer**

2:15 CHED 2009. Chemistry unbound: A complete curriculum redesign at Emory University focusing on blended learning. **D.R. Mulford**, T.L. McGill, R.J. Harris, L. Williams

2:35 CHED 2010. Gender differences and the learning outcomes in chemistry outreach. **A.M. Samani**, **P. Kamath**, **M. Rosqvist**, R.V. Valcarce, M. Alvarez, P.J. Iles, L.D. Giddings, N.R. Bastian, R. Holcomb

2:55 Intermission.

3:10 CHED 2011. New simulations for undergraduate chemistry majors. **A. Cannon**, A. Patrick

3:30 CHED 2012. Using Chem101 to enhance learning of Lewis structures and molecular shape prediction in first-year chemistry. **L. Vuocolo**, J.B. Weinberg, C. Hershock, S. Gadgil-Sharma

3:50 CHED 2013. Teaching molecular modeling at a liberal arts college before physical chemistry. **M. Paul**

4:10 Intermission.

4:25 CHED 2014. An account of continuing education in chemistry. **A. Rahman**

4:45 CHED 2015. Sleuthing through chemistry: Finding the cheapest route to a multi-step problem. **E.L. Atieh**, D.M. York

5:05 CHED 2016. Development of a non-majors chemistry course including an international travel component. **N. Beres**, **A.R. Roerdink**

Section F
New Orleans Marriott Convention Center
Blaine Kern E

Statistics & Data Management in the Chemistry Curriculum

P. Doolittle, D.G. Sykes, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 2017. Key concepts in handling big data; suggested goals for undergraduate curricula. **R. Kramer**

1:55 CHED 2018. Embedding data management into the undergraduate chemistry curriculum at James Madison University. **B.A. Reisner**, A.H. Valcourt, Y.L. Shorish

2:15 CHED 2019. Challenges to embedding statistics in the undergraduate chemistry curriculum. **N.E. Schlotter**

2:35 CHED 2020. Meeting the challenge of cloud computing: Laboratory data storage and processing. **G. Saxena**

2:55 CHED 2021. Introducing big data, statistics, R programming, and QA/QC in the analytical chemistry curriculum. **D.G. Sykes**

3:15 CHED 2022. Following phosphorus in Lake Mendota: A five year undergraduate analytical chemistry project. **P. Doolittle**

Section G
New Orleans Marriott Convention Center
Magnolia

Advancing Undergraduate Research in Chemistry: Best Practices & New Innovations

Advanced Course Integration

B.L. Gourley, *Organizer*
R.M. Jones, *Organizer, Presiding*
S. Lee, *Presiding*

1:30 CHED 2023. From procedure to practice: An organic chemsitry storyboard for developing empowered undergraduate research assistants. **N.N. Shaw**, S.B. Sigmann

1:50 CHED 2024. Incorporating research training into an advanced laboratory course. **S.M. Kennedy**

2:10 CHED 2025. Implementation of a course-based undergraduate research experience (CURE) as an organic chemistry II laboratory section. **S.K. Goforth**, H.D. Cole, E.D. Blue

2:30 CHED 2026. Reimagining biochemistry education with blended next-generation virtual laboratories. K. Hamadani, **L.A. Wirpsza**

2:50 Intermission.

3:00 CHED 2027. Engaging and training undergraduates in modern electrochemistry. **P.J. Smith**, J.C. Goeltz

3:20 CHED 2028. Integrating research-like experiences into undergraduate laboratory courses at all levels. **W. Hall**

3:40 CHED 2029. Escaping the commercial instrument paradigm in chemical education. **S. Abbott**

4:00 CHED 2030. Integration of research projects into the undergraduate chemistry curriculum. **D. Kosenkov**, Y. Kholod

Chemistry Students at the Nexus: REU Award Winners
Sponsored by PROF, Cosponsored by CHED

WCC Rising Star Award Symposium
Sponsored by WCC, Cosponsored by BIOT, CHED, COLL, INOR and PROF

Chemical Information Literacy: Innovation, Collaboration & Assessment
Sponsored by CINF, Cosponsored by CHED

Undergraduate Research in Polymer Science
Sponsored by POLY, Cosponsored by CHED and PMSE

TUESDAY EVENING

Integrating Polymer Science in the Curriculum
Sponsored by POLY, Cosponsored by CHED and PMSE

Undergraduate Research in Polymer Science
Sponsored by POLY, Cosponsored by CHED and PMSE

WEDNESDAY MORNING

Section A
New Orleans Marriott Convention Center
Blaine Kern C

Persistence in STEM: What Can we do to Support Students?

B.L. Gonzalez, *Organizer*

‡*Cooperative Cosponsorship*

S. Villafane-Garcia, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 2031. Implementation of a seminar course at a regional comprehensive institution to improve academic progress and retention. **E. Taylor**, K.S. Molek

8:55 CHED 2032. Underrepresented minority STEM organizations and science identity. **S. Nealy**, M. Orgill

9:15 CHED 2033. The Chi-Sci Scholars Program: Developing community at a minority serving institution. **K. Mardis**, M. Sabella

9:35 CHED 2034. Siena College's Tech Valley Scholars program: STEM student retention through community engaged learning. **J.L. O'Donnell**, M.W. McColgan, R.E. Kassel, S. Kellogg

9:55 Intermission.

10:10 CHED 2035. Four-year student retention and success in the Chatham University (NSF S-STEM) scholarship program. **J. MacNeil**, L. Lambert, R.B. Lettan

10:30 CHED 2036. Impact of curricular and noncurricular research involvement on STEM persistence in a primarily undergraduate institution. **B.L. Gonzalez**, A.M. Ruiz, M. Bolanos, S.R. Kdeiss

10:50 CHED 2037. Four year research engagement (FYRE) program at the University of Oklahoma: Integrating research in undergraduate curriculum. A. Burris, R.L. Halterman, A. Burgett, **N. Kothapalli**

11:10 CHED 2038. "Enhancing" general chemistry for students predicted to be at-risk. **J.R. Williams**

11:30 CHED 2039. Promoting retention in STEM by building a cohort in a summer bridge program. **J.K. Schwartz**, **C.T. Cox**, L. Andrade

11:50 CHED 2040. Impact of an alternate starting point chemistry course on success and persistence of at-risk students. **B.A. Davis**, M.A. Fisher, J.K. Vohs

12:10 CHED 2041. Students' use of online resources in preparation for general chemistry. **K.C. Smith**

Section B
New Orleans Marriott Convention Center
Blaine Kern A

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Cosponsored by CCA, LSAC, SOCED and YCC
E.J. Brush, S. Nellutla, *Organizers*
E.S. Garcia Sega, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED 2042. Development of the Dow Science and Sustainability Education Center summer research experience, a STEM education and outreach program at Saginaw Valley State University. **J. Chaytor**, D.S. Karpovich, A. Cole

9:00 CHED 2043. Why did the crystal cross the road? **J.A. Parr**

9:20 CHED 2044. The challenges and sucesses of designing experiments for CHEM CAMP and BIOCAMP, summer programs for youths 9-14. **J.B. Nielson**

9:40 CHED 2045. Counselor training model for summer chemistry camps. **R. Sansom**, D. Ess, J.B. Nielson, K.J. Stowers, J. Andersen

10:00 Intermission.

10:15 CHED 2046. Saint Francis University Rural Outreach Chemistry for Kids (R.O.C.K.) Program: Over twenty years in the making! G.C. McKernan, B. Onkst, P.T. Kasunic, R.A. Clark, **E.P. Zovinka**

10:35 CHED 2047. Closing the loop in elementary school outreach activities. **H.G. Leppert**, **Z. Crandall**, J. Swanson, J. Meyer

10:55 CHED 2048. Chemistry Ambassadors at Stanislaus State: Outreach activities and leadership skills development. **C. Reed**, **J.A. Garfield**, J. Lo, J. Godinez, P. Ayson, M. Ureño-Moreno, E.A. Aleman

11:15 CHED 2049. Beyond Benign's green chemistry outreach fellows: A multi-chapter approach to community engagement. **M.C. Enright**, D. Ward

11:35 Discussion.

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Research on Learning in the Laboratory

S. Sandi-Urena, *Organizer*
M.J. Chrzanowski, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED 2050. Student perspectives on general chemistry pre-laboratory activities. C. Tomson, **K.C. Smith**

8:55 CHED 2051. Evaluating the cognitive and affective impacts of a synthesis research project in a second-semester organic chemistry laboratory. **M. Anzovino**, M. Tsoi, A.V. Mallia, S. Park, R. Pennington, J. Sloop

9:15 CHED 2052. Development of an instrument to measure students' motivation to learn laboratory techniques. **S. Hensiek**, T.J. McCord, C.J. Harwood, M.H. Towns

9:35 CHED 2053. Analysis of diverse and independent laboratory learning environments using Langer's mindfulness theory. **M.J. Chrzanowski**, S. Sandi-Urena

9:55 Intermission.

10:10 CHED 2054. Nature of science and the general chemistry laboratory. **G. Kerstiens**, A.M. Baranger, M.C. Douskey, M. Robak, L.B. Armstrong

10:30 CHED 2055. Facilitating productive argumentation in the laboratory. **J.P. Walker**, A.G. Van Duzor, M.A. Lower

10:50 CHED 2056. Improving scientific dialogue through the evaluation of process skills. **R. Sansom**

11:10 CHED 2057. Phenomenological characterization of learning in the college chemistry laboratory. **S. Sandi-Urena**

11:30 Concluding Remarks.

Section D
New Orleans Marriott Convention Center
Blaine Kern B

Science Communication: Engaging Science Students, Scientists & Nonscientists through Modern Communication Modes

J.J. Meyers, R.H. Singiser, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 CHED 2058. Encouraging bridges: Connecting scientists and the public in the classroom, laboratory, and beyond. **L. Wysocki**, S. Mehltretter Drury

8:55 CHED 2059. Increasing science literacy in Georgia: The what, when and how of integrating literacy strategies in the STEM classroom. **C.H. Lisse**

9:15 CHED 2060. Balancing chemical equations with an interactive physical model made by 3D printing. **J.D. Mendez**

9:35 CHED 2061. What is the Venn diagram of the chemistry curriculum and the chemistry most often in the news? **T. Holme**, A. Lolinco, C. Kindle

9:55 CHED 2062. Measuring outreach: Does reading a science blog increase public engagement with science? **M. Krause**, **N.V. Hudson-Smith**, C. Allen, J.T. Buchman, E. Tollefson

10:15 CHED 2063. Developing scientific identity through a Mythbusters! style video and interaction with a local science center. **C. Lovitt**, C. Seager, J. Leibowitz

10:35 Intermission.

10:45 CHED 2064. Using YouTube videos and infographics to teach a non-majors chemistry course (Life, universe and everything: Chemistry of our daily lives). **S.P. Hickey**

11:05 CHED 2065. Impact of dynamic electronic texts on student achievement in general and organic chemistry. **J. Ross**

11:25 CHED 2066. The future of science communication is digital: Overcoming the hesitancies for online engagement. **S. Mojarad**

11:45 CHED 2067. Chemical communications at Siena College: A course in essential science communication skills. **J.L. O'Donnell**

12:05 CHED 2068. Communicating science–reactions in action and chemical etymology. **A. Basu**

12:25 Concluding Remarks.

Section E
New Orleans Marriott Convention Center
Fulton

Research in Chemistry Education

J.H. Carmel, *Organizer*
M. Anzovino, *Organizer, Presiding*
J. Carmel, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 2069. Resources to assess critical thinking, information processing, and written communication skills in undergraduate STEM courses. **G.J. Reynders**, R.S. Cole, J. Lantz, S.M. Ruder, C.L. Stanford

8:55 CHED 2070. The effect of a week-long authentic research experience on high school students' views on the nature of science. **J. Donnelly**, F. Hernandez

9:15 CHED 2071. Career selection in pre-health students at an all-male orthodox Jewish college. **J.M. Newman**, C. Sporer

9:35 Intermission.

9:50 CHED 2072. Activating potentials in chemistry education: Assessing the impact on critical thinking through active learning. **K.L. Hayden**, M. Styers, P. Van Zandt

10:10 CHED 2073. Withdrawn

10:30 CHED 2074. Comparing discipline-independent and discipline-focused metacognition in general chemistry. **K. Schnitzenbaumer**

10:50 CHED 2075. Evaluating students' retention and transfer of knowledge within a transformed chemistry curriculum for undergraduate life science majors. **C. Schnoebelen**, J.A. Chmielewski, C. Hrycyna, G.M. Bodner

11:10 Concluding Remarks.

Section F
New Orleans Marriott Convention Center
Blaine Kern E

Engaging Students in Physical Chemistry

C.M. Teague, *Organizer*
A. Grushow, *Presiding*

8:30 Introductory Remarks.

8:35 CHED 2076. Exaltation of physical chemistry: Reversing the stigma. **A.S. Frantzen**

8:55 CHED 2077. Guiding students to develop more robust knowledge structures about quantum chemical models: Translating research to practice. **M.N. Muniz**, J. Beck

9:15 CHED 2078. Using Excel VBA to promote computational thinking in physical chemistry. **G. Lo**

9:35 Intermission.

9:45 CHED 2079. Virtual reality environment to visualize and manipulate chemical interactions. J. McGraw, W. Zhang, A. Luginbuhl, G. Takahashi, R. Tasker, **G. Chopra**

10:05 CHED 2080. Molecular visualization as motivation for learning computer programming basics. **M.A. Kubasik**

10:25 CHED 2081. Computational software: Can it help increase student engagement in physical chemistry courses? **S. Nellutla**, L. Gross

10:45 CHED 2082. Development of inquiry-based physical chemistry experiments by a community of practitioners. **A. Grushow**, S.S. Hunnicutt, R.M. Whitnell, M.N. Muniz

11:05 Concluding Remarks.

Section G
New Orleans Marriott Convention

‡*Cooperative Cosponsorship*

Center
Magnolia

Advancing Undergraduate Research in Chemistry: Best Practices & New Innovations

Capstone & Community Innovations

R.M. Jones, *Organizer*
B.L. Gourley, *Organizer, Presiding*
M. Konkle, *Presiding*

8:30 CHED 2083. Undergraduate students and their role in a state certified water and soil lab. **G. Geme**

8:50 CHED 2084. Using phytoremediation to spur student interest in chemical research. **J.F. Fuller**, B.S. Arbaugh, M.A. Martin, M.E. Railing

9:10 CHED 2085. DNA-based sensors: A semester long research project as an upper-division biochemistry lab. **C.H. Battle**

9:30 CHED 2086. Conducting rigorous undergraduate student research at a small, liberal arts university: Recent progress in the investigation of the bonding and electronic structure of metal chalcogenide complexes. **J.L. Brown-McDonald**

9:50 Intermission.

10:00 CHED 2087. Training undergraduates to design research projects: Innovations and activities in a senior capstone course. **J.M. Wiester**

10:20 CHED 2088. Design and implementation of a research-based laboratory capstone course built around discovery, collaboration, and the integration of the chemistry sub-disciplines. **J.A. MacKay**

10:40 CHED 2089. Designing a chemistry laboratory program for a research-focused ACS-approved curriculum. **A.O. Sezer**

11:00 CHED 2090. Developing an integrated research and learning model that aid students and faculty. **R.E. Bachman**

WEDNESDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
Blaine Kern C

Persistence in STEM: What Can we do to Support Students?

S. Villafane-Garcia, *Organizer*
B.L. Gonzalez, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 2091. Arithmetic skills and algebraic competency for STEM advancement. **D.S. Mason**

1:55 CHED 2092. Impacting retention of STEM freshmen and transfer students through research communities within the LEARN Consortium. **D. Chamely Wiik**, **W.R. Kwochka**

2:15 CHED 2093. Designing and implementing a dashboard to monitor mentor performance for a STEM persistance program. **A. Ma**, **K. Gerald**, W. Colon

2:35 CHED 2094. Cyber mentoring to increase persistence for students in STEM. **G.M. Korenowski**, A. Ma, W. Colon

2:55 CHED 2095. Early college exposure to non-tenure track and part-time faculty – Examining effects on socialization and student success in science, technology, engineering, and mathematics. **K. Van Kirk**, R. Franke

3:15 Intermission.

3:30 CHED 2096. Foundational mathematics knowledge and persistence in general chemistry. **R.J. Weber**

3:50 CHED 2097. Withdrawn

4:10 CHED 2098. VOICES: Voluntary options in chemical education schedules. R.L. Ford, S. Broadway, **D.S. Mason**

4:30 CHED 2099. Impact of an emerging gateway course model at the University of Southern Maine. **L. Benedict**, P. Dexter

4:50 CHED 2100. Contextualizing STEM with first year transdisciplinary laboratories. **R.N. Dansby-Sparks**, S. Formica, M. Smith

Section B
New Orleans Marriott Convention Center
Blaine Kern A

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Cosponsored by CCA, LSAC, SOCED and YCC
E.J. Brush, E.S. Garcia Sega, S. Nellutla, *Organizers*
S. Nellutla, *Presiding*

1:30 Introductory Remarks.

1:40 CHED 2101. Syracuse University's summer chemistry enrichment experience – development of an outreach pilot program. **G. Bonomo**, B. Kunnath, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

2:00 CHED 2102. Leveraging teacher partnerships to facilitate effective high school visits and mentorship. **S. Iyer**, **J.K. Schwartz**

2:20 CHED 2103. Sustainability education and outreach to promote diversity in the STEM workforce. **J. Blatti**

2:40 CHED 2104. Fighting with food, battling chemical toxicity with good nutrition: Outreach to teachers and students and student outreach to their peers. **S.A. Hershberger**

3:00 Intermission.

3:15 CHED 2105. Chemistry in the community: Service learning for Tulane students in New Orleans. **R. Vik**, **E. Schmidt**, C.H. Battle, J. Jayawickramarajah

3:35 CHED 2106. Chemistry in the community: Developing community partners in New Orleans. **C.H. Battle**, R. Vik, E. Schmidt, J. Jayawickramarajah

3:55 CHED 2107. Service learning in the chemical sciences: A few insights. **S.M. Grayson**, H. Ashbaugh

4:15 CHED 2108. Service-learning programs for chemistry majors and general education students. **T.D. Hamilton**

4:35 Discussion.

4:45 CHED 2109. CHEM – STEM with exploring, learning, and mentoring. **M. Rustagi**

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Eye Tracking Research in Chemistry Education

S.J. Hansen, *Organizer*
J.R. Vandenplas, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED 2110. Measuring student visual attention to conceptual and algorithmic information in general chemistry worked examples. **E. Day**, L.K. Kendhammer, N.J. Pienta

1:55 CHED 2111. Use of eye tracking and verbal articulation to understand students' decision-making processes when solving high-stakes assessment items. J.J. Reed, J.M. Trate, D. Schreurs, J.R. Raker, **K.L. Murphy**

2:15 CHED 2112. Visual feedback and animation critique. **S.J. Hansen**, B. Hu, D. Riedlova

2:35 CHED 2113. Modeling split attention during simulation use. **J.R. Vandenplas**, D.G. Herrington, R.D. Sweeder

2:55 Intermission.

3:00 CHED 2114. Optimizing STEM skills: Understanding the allocation of attention during mental rotation. **M. Beck**, K. Moen, S. Greening, L.G. Butler, J. Ramanujam, A. Cohen

3:20 CHED 2115. Measuring the cognitive load of modeling activities in chemistry. **K.J. Linenberger Cortes**, A. Randolph, C. Terrell, X. Prat-Resina, K. Kammerdiener, J. Calvert, L. Aleuy, J. Farmer

3:40 CHED 2116. Eye tracking with organic chemistry reaction mechanisms. **M. Weinrich**

4:00 Concluding Remarks.

Section D
New Orleans Marriott Convention Center
Blaine Kern B

There's an App for That!

E.A. Aleman, K. Stone, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 CHED 2117. ARiEL: Augmented reality in the educational laboratory. **T. Holme**, P. Laila-Parvin

1:55 CHED 2118. iPad technology in the organic chemistry classroom. **J.L. Marshall**

2:15 CHED 2119. Developing and implementing Tap OChem, an organic chemistry app, for small and large classroom use. **N.T. Allison**

2:35 CHED 2120. Role of chemistry apps in teaching general chemistry at Bridgewater State University. **S. Nellutla**

2:55 Intermission.

3:10 CHED 2121. Going paper-free and facilitating collaboration through the use of iPads as electronic laboratory notebooks in an advanced chemistry laboratory course. **J. Fishovitz**, K.L. Haas

3:30 CHED 2122. Creating a digital laboratory notebook for mobile devices. **A.R. Van Dyke**, J.E. Smith-Carpenter

3:50 CHED 2123. A paperless physical chemistry laboratory. **E.A. Aleman**

4:10 CHED 2124. Less grading time for you: More writing and learning for your students. **K. Stone**

4:30 Concluding remarks.

Section E
New Orleans Marriott Convention Center
Fulton

General Papers

S.A. Fleming, *Organizer*
J. Statler, *Presiding*

1:30 Introductory Remarks.

1:35 CHED 2125. Innovative project design with microwave technology in undergraduate teaching labs. **G. Dusharm**, M.J. Karney

1:55 CHED 2126. Expanding the tool box in undergraduate laboratory sessions via continuous flow synthesis. **V. Kairouz**, J. Santandrea, S.K. Collins

2:15 CHED 2127. Laboratory-based project in a lecture-only inorganic chemistry course. **K.M. Krise**

2:35 CHED 2128. Microscale extraction of liquid oxygen from a cryogenic mixture fomred through condenstaion of ambient air. **J. Statler**

2:55 Intermission.

3:10 CHED 2129. A 3-D nanoscience lesson based on NGSS standards implemented at Towson University. **M. Devadas**, D. Menon

3:30 CHED 2130. New demonstration with BZ chemical oscillator. **G.A. Frerichs**, G. Ali

3:50 CHED 2131. Withdrawn

4:10 Intermission.

4:25 CHED 2132. Revising a classic general chemistry lab to introduce green chemistry principles. **S.J. Bachofer**, M.D. Lingwood

4:45 CHED 2133. History of science, a transcultural student experience: Design, implementation, evaluation and future directions. **R. Morgan Theall**, **C. Ragain**, J. Kessler, C. McGowan

5:05 CHED 2134. Hands-on 3D printed models of atomic and hybrid orbitals. R. De Cataldo, K. Griffith, **K.H. Fogarty**

Section F
New Orleans Marriott Convention Center
Blaine Kern E

Engaging Students in Physical Chemistry

C.M. Teague, *Organizer*
A. Grushow, *Presiding*

1:30 Introductory Remarks.

‡*Cooperative Cosponsorship*

1:35 CHED 2135. Introducing the chemistry of molten salts in the nuclear engineering curriculum. **R.O. Scarlat**

1:55 CHED 2136. Building tomorrow's scientists: A guided research project to build the research and soft skills every scientist needs for a successful career. **A. Bills**

2:15 CHED 2137. Short introductory activities for physical chemistry laboratory. **G. Lo**, D. Wayment, C. Dong

2:35 Intermission.

2:45 CHED 2138. Enhancing meaningful learning opportunities in the physical chemistry laboratory despite limited resources. **A.L. Smalley**

3:05 CHED 2139. Toward the characterization of student learning outcomes in POGIL-PCL laboratory environments. **M.N. Muniz**, B. Tyler, S.S. Hunnicutt, R.M. Whitnell, A. Grushow

3:25 CHED 2140. Updating a classic: Using absorption spectroscopy of diatomic molecules to highlight the similarities and differences of diatomic potential energy curves. **K.S. Dooley**

3:45 Concluding Remarks.

Section G
New Orleans Marriott Convention Center
Magnolia

Advancing Undergraduate Research in Chemistry: Best Practices & New Innovations

Department & Institutional Innovations

B.L. Gourley, *Organizer*
R.M. Jones, *Organizer, Presiding*
R.E. Bachman, *Presiding*

1:30 CHED 2141. Bringing undergraduate research to a crescendo: Project Symphony at Iona College. **S. Lee**

1:50 CHED 2142. "*Opportunitas*": Pace University approach in innovating undergraduate research program. **E.E. Mojica**

2:10 CHED 2143. Undergraduate research as a transformative student experience and a tool to increase student retention. **M.R. Harris**

2:30 CHED 2144. Knowing your colleagues: The importance of vertical and horizontal cohorts to the success of undergraduate research. **D.F. Moriarty**, L.J. Tucker

2:50 CHED 2145. Successful research models for undergraduates at a small public institution. **A.G. Cavinato**

3:10 Intermission.

3:20 CHED 2146. From chemistry specific to institution wide: Establishing an Office of Undergraduate Research. **M. Richards-Babb**

3:40 CHED 2147. Best practices at the West Virginia University Department of Chemistry Research Experiences for Undergraduates site. **B.V. Popp**, M. Richards-Babb

4:00 CHED 2148. DIVAS: A common challenge approach to interdisciplinary research. **R.M. Burks**, T. Durham-Brooks, M. Meysenburg

4:20 CHED 2149. Using undergraduate research to enhance STEM education at the departmental and institutional Level. **M.R. Malachowski**, K.K. Karukstis

4:40 CHED 2150. Investigating impacts of authentic environmental research experiences in the college classroom: A multi-institution collaboration to incorporate research throughout the curriculum and across disciplines. **J.H. Tomasik**, D.J. Lecaptain, A. Mueller, T. Sivy, D.S. Karpovich, K. Cissell, B.S. Harkness, J. VanHouten

5:00 Concluding Remarks.

THURSDAY MORNING

Section A
New Orleans Marriott Convention Center
Blaine Kern C

Persistence in STEM: What Can we do to Support Students?

S. Villafane-Garcia, *Organizer*
B.L. Gonzalez, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CHED 2151. Students' chemistry self-efficacy: Exploring its relationship with their sources, teaching and learning in a general chemistry course. **S. Villafane-Garcia**

8:25 CHED 2152. Targeting and preparing at-risk students: Increasing success in 1st semester general chemistry. **K.L. Stone**, **S.E. Shaner**, C.M. Fendrick

8:45 CHED 2153. Partial least squares structural equation modeling of chemistry attitudes in introductory college chemistry. **J. Ross**, L. Nuñez, C. Lai

9:05 CHED 2154. What is the relationship between a students' profile and their success on common questions in first-semester general chemistry? **V.M. Williamson**

9:25 CHED 2155. The impact of a group-testing protocol on student test anxiety and test performance in a general chemistry course at the University of Washington. **M. Mack**, C. Craig, S. Freeman

9:45 Intermission.

10:00 CHED 2156. A survey instrument for measuring the persistence and quality of life of chemistry graduate students. **E.T. Novelli**, L.J. Webb

10:20 CHED 2157. Persisting without calculators. **D.R. Walker**

10:40 CHED 2158. Developmental coursework as a needed path to STEM success. **B. Mamiya**, A. Chen, **D.S. Mason**, C. Zajac

11:00 CHED 2159. A fifteen-year retrospective analysis of achievement gaps in chemistry education at the University of Washington. **M. Mack**, R. Harris, S. Freeman, E. Theobald, J. Bryant

11:20 CHED 2160. Mathematics competency of males and females in general chemistry and STEM retention. **G.R. Shelton**

Section B
New Orleans Marriott Convention Center
Blaine Kern A

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Cosponsored by CCA, LSAC, SOCED and YCC
E.S. Garcia Sega, S. Nellutla, *Organizers*
E.J. Brush, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 CHED 2161. Enhnacing MRSEC education outreach with STEM on Stage video. **D. Steinberg**, C.B. Monroe, S. Rodriguez Martinez, J. Myronuk

8:30 CHED 2162. End of an era: Lessons learned from 10 years of uutreach at a NSF-funded center. **J.D. Schuttlefield Christus**, M. DeBoever

8:50 CHED 2163. West Virginia Brigade of the Solar Army: Renewable energy outreach through Fairmont State University. **A.R. Moore**, **S. Starcovic**, **E.L. Harvey**

9:10 CHED 2164. Combining sustainability and polymers: Physical science curriculum for informal K-8 science audiences. **J. Henderson**, A. Stevenson, A. Maille, C. Malone, M. Smith, S. Worker

9:30 CHED 2165. *Caminos a la Ciencia*/Pathways to Science: An innovative NSF-INCLUDES program designed to attract and engage Hispanic girls in STEM inquiry in the central Virginia region. **A. Marchetti**

9:50 Intermission.

10:05 CHED 2166. ChemAttitudes: Developing and disseminating strategies and materials to support chemistry interest, relevance, and self-efficacy. **D.F. Sittenfeld**, M.M. Kirchhoff, L. Bell, E. Kollmann, R. Ostman

10:25 CHED 2167. Using design-based research to learn about strategies that increase feelings of interest, relevance, and self-efficacy in chemistry. **M. Beyer**, E. Kollmann, M. Bequette, S. Pfeifle, K.T. Povis, G. Haupt

10:45 CHED 2168. Symposium workshop on the fundamentals of chemistry outreach education: II. Finding Resources. **E.J. Brush**, **E.S. Garcia Sega**, **S. Nellutla**

11:25 Concluding Remarks.

Section C
New Orleans Marriott Convention Center
Tchoupitoulas

Chemistry Safety in the Classroom: Best Practices & Learning Experience

S.D. Wiediger, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CHED 2169. PubChem's health and safety information for laboratory chemicals. **S. Kim**, J. Zhang, A. Gindulyte, P. Thiessen, L. McEwen, R. Stuart, E. Bolton

8:25 CHED 2170. Risk analysis is not a guessing game especially for classroom demostrations. **D.J. Leggett**

8:45 CHED 2171. Withdrawn

9:05 Intermission.

9:20 CHED 2172. Drawing your way to safety: Diagramming the laboratory's layout and safety equipment. **J.M. Newman**, A.E. Shinnar

9:40 CHED 2173. Undergraduate and TA knowledge and implementation of safety guidelines in the general chemistry laboratory. **H. Broussard**, N.J. Pienta

10:00 CHED 2174. Incorporating active learning into safety training. **C.T. Cox**

10:20 CHED 2175. Adding safety to the curriculum one research project after another. **S.D. Wiediger**

10:40 Concluding Remarks.

Section D
New Orleans Marriott Convention Center
Blaine Kern B

Using Videos in Teaching

J.A. Parr, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CHED 2176. Integration of digital videos into student learning experiences. **R.E. Belford**

8:20 CHED 2177. Creating custom course videos as the content backbone for general chemistry courses. **M.A. Deri**, D.M. McGregor, P. Mills

8:35 CHED 2178. Withdrawn

8:50 CHED 2179. Preparing students for class using videos. **J.A. Parr**

9:05 CHED 2180. YouTube as an open educational resource (OER) hosting general and organic chemistry course videos: Creating an online footprint while evaluating locally enrolled student engagement. **D. Jackson**

9:20 Intermission.

9:30 CHED 2181. Exploring the use of SMART Boards: Creating a blended learning environment for organic chemistry courses by producing multimedia lessons and videos using an interactive white board. **M. Chatterjee**

9:45 CHED 2182. Putting it all together: Creation of a YouTube channel for organic chemistry screencasts and videos. **M.G. Donahue**

10:00 CHED 2183. Use of multi-media tools in the chemistry classroom to foster student participation. **R. Broyer**

10:15 CHED 2184. The impact of student-created mechanism videos in organic chemistry-2 labs. **N. Gupta**, J.A. Nikles

10:30 CHED 2185. Creating videos and animations to enhance organic chemistry lecture and laboratory instruction. **L. Starkey**

10:45 Intermission.

10:55 CHED 2186. Using videos in teaching nmr processing. **C.M. Bump**, G.C. Nwokogu, E.N. Ndip, M.K. Waddell, M. Malik

11:10 CHED 2187. Flipped quantitative analysis. **R.L. Sanders**

11:25 CHED 2188. Use of videos in enhancing the teaching and learning of chemistry in lecture and laboratory classes. **E.E. Mojica**, R.K. Upmacis

‡*Cooperative Cosponsorship*

11:40 CHED 2189. Using Game of Thones, Nicolas Cage and Harry Potter (amongst others) to teach biochemistry to non-science majors. **S.P. Hickey**

11:55 Concluding Remarks.

Section E
New Orleans Marriott Convention Center
Fulton

Research in Chemistry Education

M. Anzovino, J.H. Carmel, *Organizers*
D. Behmke, S. Srinivasan, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 2190. Response process validity evidence of an immediate feedback assessment. **J.M. Trate**, S. Srinivasan, T.S. Thomas, C.J. Luxford, M.A. Teichert, J.L. Schneider, K.L. Murphy

8:25 CHED 2191. Investigation of general chemistry assessment item stability: Same items, different form – what changes? **T.C. Pentecost**, J.R. Raker, K.L. Murphy

8:45 CHED 2192. When is the optimum time to measure affect?: The impact of examination performance and feedback on affect in organic chemistry courses. **J.R. Raker**, R. Gibbons

9:05 CHED 2193. Withdrawn

9:25 Intermission.

9:40 CHED 2194. Assessment in postsecondary chemistry education: Results from a national survey. R. Gibbons, K.L. Murphy, **J.R. Raker**

10:00 CHED 2195. Faculty conceptions and use of writing as a pedagogical tool in chemistry. **S.A. Finkenstaedt-Quinn**, A. Moon, J. Dowd, A. Gere, G.V. Szymczak

10:20 CHED 2196. Peer-led team learning (PLTL) use in postsecondary chemistry education: Results from a national survey. **S. Srinivasan**, R. Gibbons, J.J. Reed, K.L. Murphy, J.R. Raker

10:40 Concluding Remarks.

Section F
New Orleans Marriott Convention Center
Blaine Kern E

General Papers

S.A. Fleming, *Organizer*
R. Indralingam, *Presiding*

8:00 Introductory Remarks.

8:05 CHED 2197. Development of green multistep synthesis for undergraduate organic laboratory. **A.N. Lamm**

8:25 CHED 2198. Experimental determination of activation energy of nucleophilic aromatic substitution on porphyrins. **C.M. Drain**, W. Rizvi, E. Khwaja, S. Siddiqui, N.K. Bhupathiraju

8:45 CHED 2199. Withdrawn

9:05 CHED 2200. Developing a viable organic chemistry research project for ACS SEED. T. Davis, H. Allen, J. Hood, M.G. Donahue, **J.A. Pigza**

9:25 Intermission.

9:40 CHED 2201. Teaching students to apply core biochemical concepts to practical goals by completing authentic course-based research projects organized online. **B.J. McFarland**

10:00 CHED 2202. Putting the carbonyl cart before the substitution horse: A new approach to teaching sophomore organic chemistry. **J.K. Murray**, M.J. Castaldi

10:20 CHED 2203. Fluorometric monitoring of the photodegradation of riboflavin. **R. Indralingam**, S.O. Ali

10:40 CHED 2204. Adapting cell-free protein synthesis as a platform technology of biochemical education. **J.P. Oza**, N.E. Gregorio, W.Y. Kao, M.C. Jewett

Section G
New Orleans Marriott Convention Center
Magnolia

Online & Upward: Improving Online Education to Increase Chemistry's Global Reach

M.A. Erdmann, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CHED 2205. Experiences with online chemistry education: Understanding the challenges. **E. Pearsall**

8:25 CHED 2206. Growing up online: Building a general chemistry course with lab from experiences collected over seven years of delivering a non-majors chemistry course with lab online. **S. Burchett**, **J.L. Hayes**

8:45 Intermission.

9:00 CHED 2207. A new interactive, 3D chemistry learning and teaching platform. **A. Cannon**, A. Patrick

9:20 CHED 2208. WileyPLUS an online chemistry homework system powered by Marvin JS a state of the art web based chemical drawing tool. **A.D. Costache**, E.A. Hoffmann, S. Bruno, S.P. Hickey

9:40 CHED 2209. Three approaches to supporting online learners in lab-based chemistry courses. **K.L. Kostka**

CHAS

Division of Chemical Health and Safety

D. Decker and J. Pickel, *Program Chairs*

OTHER SYMPOSIA AND WORKSHOPS OF INTEREST:

CHAS Workshop: Lab Safety, 8:30 AM: Fri

CHAS Workshop: Laboratory Waste Management, 8:30 AM: Fri

CHAS and CANN Workshop: How to be a More Effective Chemical Hygiene Officer, 8:30 AM: Sat

CHAS and CANN Workshop: Reactive Chemical Management for Laboratories & Pilot Plants, 8:30 AM: Sat

CHAS and CANN Workshop: Cannabis Extraction & Analysis, 8:30 AM: Sat

CHAS/CCS Workshop: Developing Graduate Student Leadership Skills in Laboratory Safety, 3:00 PM: Sun

BUSINESS MEETINGS:

CHAS Board Meeting, 8:00 AM: Sun

SUNDAY MORNING

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

SUNDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 21

Ask Dr. Safety: Integrating Research & Safety
Cosponsored by CCS
N.R. Langerman, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHAS 1. The psychology of developing a positive chemical safety culture in academic research labs. **K.A. Serrano**

2:00 CHAS 2. Survey of chemist exposure to VOCs from solvent cabinets. **A.E. Norton**, W.B. Connick, K. Brown

2:25 CHAS 3. Study of safer storage and handling of graphene oxide. **P. Lakhe**, D. Kulhanek, W. Sun, B. Zhang, M.J. Green, S. Mannan

2:50 CHAS 4. Effectiveness of laser safety eyewear under real-world conditions. **C.J. Stromberg**, E.J. Heilweil, J.A. Hadler

3:15 CHAS 5. Safety at the bench: Promoting positive safety culture in academic laboratories. **C.N. Situma**

3:40 CHAS 6. Ask Dr. Safety: Integrating research and safety. **N.R. Langerman**, H.J. Elston

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

MONDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 21

Women in Cannabis: Shaping an Emerging Industry
Cosponsored by SCHB‡ and WCC
Financially supported by CANN
M.J. Wilcox, *Organizer*
M. Wilcox, *Presiding*

8:30 Introductory Remarks.

8:35 CHAS 7. Moving an industry forward: How women are shaping the future of cannabis. **M.J. Wilcox**

9:00 CHAS 8. Evolution of the cannabis industry: an outside view from the inside. **A. Rigdon**

9:25 CHAS 9. Movement toward consensus analytical test methods and standards for the cannabis community to ensure consistent product characterization. **S.A. Audino**

9:50 CHAS 10. Withdrawn

10:15 Intermission.

10:30 CHAS 11. Cleaning up cannabinoids and chlorophyll: Optimization of sample preparation for pesticide analysis in cannabis flower. **J. Kowalski**, D. Laine, S. Minier, C. Johnson

10:55 CHAS 12. Sex differences in clinical pharmacology and gender differences in society: How to give an emerging industry a head start. **L. Klumpers**

11:20 CHAS 13. Roadblocks, guardrails & opportunities. **T. Wahl**

11:45 CHAS 14. Transitioning from academia to cannabis: Why chemists and their influence are important contributors to a growing industry. **A.R. Wise**

12:10 Panel Discussion.
12:30 Concluding Remarks.

Community Sharing of Chemical Safety Data: Yes, No, Maybe?
Sponsored by CINF, Cosponsored by CHAS, CA and PRES‡

MONDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 21

Implementing ACS Safety Education Guidelines
Cosponsored by CCS and CHED
Financially supported by AACT
E.M. Howson, *Organizer*
S.B. Sigmann, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHAS 15. The ACS safety culture journey: What next? **M.U. Gmurczyk**, **M.M. Kirchhoff**

2:05 CHAS 16. Building the safety learning spiral. **R. Stuart**, S.B. Sigmann

2:25 CHAS 17. One slice at a time: Do what you can whenever you can. **K.P. Fivizzani**

2:45 CHAS 18. Developing a culture of safety in chemistry and biochemistry at Texas Woman's University. **R.D. Sheardy**

3:05 Intermission.

3:25 CHAS 19. Importance of laboratory safety in chemistry curriculum. **K. Jefferson**

3:45 CHAS 20. Impact of implementing the RAMP concept for chemical safety training in undergraduate teaching. **O. Oluwaniyi**

4:05 CHAS 21. RAMPing up the organic chemistry lab at a PUI: Developing a culture of safety and success. **R.S. Majerle**, M. Gorina

MONDAY EVENING

Section A
Ernest N. Morial Convention Center

‡*Cooperative Cosponsorship*

Halls D/E

Sci-Mix
J.M. Pickel, *Organizer*
8:00–10:00

CHAS 22. Division of Chemical Health and Safety information poster. **J.M. Pickel**

CHAS 23. Rapid chemical risk assessments for research labs. **D.J. Leggett**

CHAS 24. Femtosecond laser eyewear protection: Measurements and precautions. **M. Riedel-Topper**, **S. Wirick**, J.A. Hadler, E.J. Heilweil, C.J. Stromberg

CHAS 25. Workshop for high school chemistry teachers on case studies of K-12 lab accidents and safety resources. **C. Lilly**

CHAS 26. A flexible web-interface for integrating multiple data streams in support of risk prioritization of environmental chemicals. R. Judson, A.J. Williams, **C. Grulke**, R. Thomas

CHAS 27. Evaluation of cannabinoid and terpene interference in HPLC-UV cannabis potency testing. **A. Rigdon**, C. Sweeney, C. King, B. Cassidy, J. Kowalski, F.L. Dorman

CHAS 28. Health risk of oral and inhalation exposure to toxic chemicals. **A. Fontenot**, H. Hwang

TUESDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 21

Water Supply Safety
Cosponsored by CCS, CTA and ENVR
M.R. Wilhelm, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 CHAS 29. Waukesha water: Bridging the divide. D. Duchniak, **J. Piatt**

9:30 CHAS 30. Laboratory safety is impacted by changes in water quality. **C. Wilhelm**

9:55 CHAS 31. Iron as an indicator of water system corrosion and compromised disinfection: Argument for regulating iron and small system corrosion control. **A. Katner**, K. Pieper, M. Edwards

10:20 CHAS 32. Lessons learned from the Elk and Dan River disasters: Enhancing science support for water resource protection and crisis communication in spill-incident response. **W.A. Alexander**

10:45 CHAS 33. Computational chemistry support for water resource protection: Developing rapid and accurate computational methods to predict physical properties for environmental fate and toxicity modelling. **K. Charbonnet**, N.J. Deyonker, W.A. Alexander

11:10 Panel Discussion.

Biobased Water Purification System Approaches
Sponsored by CELL, Cosponsored by AGFD, CHAS and ENVR

TUESDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 21

Formulation of Cannabis Products: More than just THC & CBD

Financially supported by CANN
M. Roggen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHAS 34. At-line to on-line cannabis extraction and isolaton. **J. MacKay**

2:05 CHAS 35. Analytical procedures and specifications for a Cannabis based prescription drug. **P. Gibson**, A. Sutton, A. Silcock

2:35 CHAS 36. Controlling terpenes and cannabinoids in flower and extract. **M. Roggen**

3:05 Panel Discussion.
3:25 Intermission.

3:45 CHAS 37. Does 1+1=3? What science really knows about cannabinoid and terpene effects in humans. **L. Klumpers**, K. Franson

4:15 CHAS 38. In search of efficacy: A self-reported patient study identifying effective THC:CBD ratios for sleep, pain and arousal based on dose-controlled delivery of vaporized cannabis oil. **S.J. Miller**

4:45 CHAS 39. Potential health risks of cannabis extracts. **T. Lewandowski**, J. Rice

5:15 Panel Discussion.
5:25 Concluding Remarks.

Science & Ethics: The Path Toward Global Security in Chemicals, Energy, Food & Water
Sponsored by SCHB, Cosponsored by CHAS, COMSCI, MPPG and PROF

Evolving Chemical Hazard Evaluation Strategies to Address Compliance under the New Toxic Substances Control Act (TSCA)
Sponsored by ENVR, Cosponsored by CHAL and CHAS

WEDNESDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 21

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Cosponsored by AGFD, CHAL and SCHB
Financially supported by CANN
E.M. Pryor, *Organizer, Presiding*
A. Pham, *Presiding*

9:00 Introductory Remarks.

9:05 CHAS 40. Shaping the bright future of the cannabis industry: Because we can. **L. Klumpers**, D.L. Thacker, K. Franson

9:40 CHAS 41. The identification of Δ-8 tetrahydrocannabinolic acid (Δ-8-THCA) by NMR and LCMS techniques. **M. Scialdone**, C. Barone, C. Rithner, K. Denef, C. Boot

10:15 CHAS 42. Chemistry of Canadian medical cannabis. **M.M. Lewis**, Y.W. Yang, E. Wasilewski, H. Clarke, L.P. Kotra

10:50 CHAS 43. Heidolph North America's Cannabis Chemistry Scholarship in it's first of many years: What to expect for the future of CANN and "CANNCHASHNA" scholarship. **E.M. Pryor**, J. Marcu, A. Pham, M.J. Wilcox, E.L. Oltermann

11:25 Pannel Discussion.

WEDNESDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 21

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Cosponsored by AGFD, CHAL and SCHB
Financially supported by CANN
E.M. Pryor, *Organizer, Presiding*
A. Pham, *Presiding*

1:30 Introductory Remarks.

1:45 CHAS 44. Analysis of regulatory improvements and setbacks for medical cannabis programs and product safety standards. **J. Marcu**, S. Sherer

2:20 CHAS 45. Adventures in the Cannabis field: Surprises and discoveries with natural and synthetic cannabinoids. **M.A. Schafroth**, R. Sarott, E. Carreira

2:55 CHAS 46. THC and its metabolites in blood: Legal, regulatory, and scientifi challenges in the context of cannabis DUI. **A. Pham**, E.M. Pryor

3:30 CHAS 47. Rapid metabolic phenotyping of a medicinal plant: Applications for C. Sativa. **J. de la Parra**, E. Anemone, F. Jackson, w. Hancock, J. Auclair

4:05 Panel Discussion.

THURSDAY MORNING

Separation Science & Technology in the Medical Cannabis & Hemp Industry
Sponsored by I&EC, Cosponsored by CHAS

Separation Science & Technology in the Medical Cannabis & Hemp Industry
Sponsored by I&EC, Cosponsored by CHAS

CINF

Division of Chemical Information

E. Alvaro and R. Bienstock, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Jürgen Bajorath (see *COMP*, Tue)

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences (see *COMP*, Sun, Mon)

Open Resources for Automated Structure Verification & Elucidation (see *ANYL*, Sun)

Structure-Based Drug Design for GPCRs (see *COMP*, Wed)

BUSINESS MEETINGS:

Business Meetings, 12:30 PM &
3:00 PM: Sat

SUNDAY MORNING

Section A
New Orleans Marriott Convention Center
River Bend 1

Enhance Discovery: Share Chemical Structures

Financially supported by Chemical Structure Association Trust
Y. Li, V.F. Scalfani, *Organizers*
L. McEwen, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CINF 1. Sharing chemical structures from university theses and dissertations on Institutional Repositories and PubChem. **V.F. Scalfani**, P. Rupar, M.S. Alexander, D.G. Williams

9:05 CINF 2. Impact of Stereochemistry on Sharing Chemical Structures. **G.M. Banik**, M. Karthikeyan, K. Nedwed, K. Kunitsky, M. D'Souza, T. Abshear

9:30 CINF 3. Sharing chemical data through a structural database. **S. Ward**, A. Sarjeant, I. Bruno, M.P. Lightfoot

9:55 Intermission.

10:10 CINF 4. Deposit chemical structures into PubChem–a public data repository. **J. Zhang**, A. Gindulyte, B. Shoemaker, P. Thiessen, E. Bolton

10:35 CINF 5. Supporting the community to share chemical structures. **G. Jones**, R. Kidd

11:00 CINF 6. Chemical structures: More than just meta-data? **M.G. Hicks**

11:25 Discussion.

Section B
New Orleans Marriott Convention Center
Natzhez

Drug Discovery: Cheminformatic Approaches
Cosponsored by COMP
E. Davis, *Organizer, Presiding*

9:00 CINF 7. Synthetically Accessible Virtual Inventory (SAVI) – Next version: Toward more needles and less haystack. **H. Patel**, Y. Pevzner, W. Ihlenfeldt, M.C. Nicklaus

9:25 CINF 8. BioTransformer: An accurate, freely available tool for predicting small molecule metabolism–Applications in drug discovery. **Y. Djoumbou Feunang**, D. Wishart

9:50 CINF 9. CCCTK (Compute Cure for Cancer ToolKit): An open source drug discovery platform for design of novel anti-cancer agents. **M. Karthikeyan**, R. Vyas

10:15 Intermission.

10:30 CINF 10. Practical machine learning methods for QSPR and QSAR predictions. **V. Tkachenko**, A. Korotcov, R. Zakharov, B. Sattarov, A. Mitrofanov

10:55 CINF 11. Making virtual REAL: synthetically feasible compounds and their exploration in docking screens. **Y. Moroz**

‡*Cooperative Cosponsorship*

11:20 CINF 12. Deep learning approaches for detecting high-throughput screening false positives. **M. Matlock**, T. Hughes, S. Swamidass

11:45 CINF 13. Virtual screening and fast resynthesis of hits: Anchor.Query. **A. Doemling**, D. Koes, C.J. Camacho

Drug Design

Structure & Ligand-Based Design

Sponsored by COMP, Cosponsored by CINF

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Data Mining & Frameworks for Chemical Discovery

Sponsored by COMP, Cosponsored by CINF and PHYS

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

SUNDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
River Bend 1

Enhance Discovery: Share Chemical Structures

Financially supported by Chemical Structure Association Trust
L. McEwen, *Organizer*
Y. Li, V.F. Scalfani, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 CINF 14. Sharing chemical structures with peer-reviewed publications. Are we there yet? **A.J. Williams**

1:35 CINF 15. Integration of Markush structures into EPA's DSSTox database to represent and enumerate UVCB substances. **C. Grulke**, A.J. Williams, A. Richard

1:55 CINF 16. Curating and sharing structures and spectra for the environmental community. **E. Schymanski**, A.J. Williams

2:15 CINF 17. ChemAxon's chemical structure file formats for better data storage and search. **A.D. Costache**, E.A. Hoffmann, A. Volford

2:40 CINF 18. NCI/CADD CACTUS web server: Tool for connecting chemical structures. **M.C. Nicklaus**

3:05 Intermission.

3:20 CINF 19. Sharing chemical structures: Workflows, demonstrations, and discussion. **V.F. Scalfani**, **L. McEwen**, **Y. Li**, **E. Schymanski**, **A. Costache**, **E.A. Hoffmann**, **A. Volford**, **A.J. Williams**, **C. Grulke**, **J. Zhang**, **S. Ward**, **G. Jones**, **G.M. Banik**

Section B
New Orleans Marriott Convention Center
Natzhez

Fragrances, Food & Cheminformatics

R.J. Bienstock, J.A. Bikker, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 CINF 20. Global structure diversity and chemical space of food chemicals. N.N. Trujillo-Minero, **J.L. Medina-Franco**

1:40 CINF 21. Food additives data integration in PubChem. **J. Zhang**, P. Thiessen, A. Gindulyte, E. Bolton

2:00 CINF 22. Using structural data in the food and fragrance industries. **S. Ward**, A. Sarjeant, S. Vyas, P.I. Andrews

2:20 Intermission.

2:30 CINF 23. Predicting human olfactory perception from molecular structure. **J. Mainland**

2:50 CINF 24. Using molecular fields to understand molecular determinants of the olfaction process. **M. Slater**

3:10 CINF 25. Withdrawn

3:30 CINF 26. QSAR/QSPR models to support fragrance ingredient molecular design. D. Chekmarev, J. Kattas, **J.A. Bikker**

3:50 Intermission.

4:00 CINF 27. Translating methods from pharma to fragrances and flavors. **T. Mansley**, E. Champness, P. Hunt, N. Foster, **M.D. Segall**

4:20 CINF 28. Predicting color stability of fragrance ingredients in consumer products based on molecular structure. D.T. Stanton, **P.J. Madhav**

4:40 CINF 29. Computational analysis towards understanding food dye and coloring agent genotoxicity. **R.J. Bienstock**, L. Perera, M.A. Pasquinelli

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Artificial Intelligent Searching of Chemical Space

Sponsored by COMP, Cosponsored by CINF and PHYS

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY MORNING

Section A
New Orleans Marriott Convention Center
River Bend 1

Community Sharing of Chemical Safety Data: Yes, No, Maybe?
Cosponsored by CHAS, CA and PRES‡
C.I. Nitsche, *Organizer, Presiding*

8:20 CINF 30. What's all this fuss about data sharing? In search of improved laboratory safety. **C.I. Nitsche**

8:30 CINF 31. Promoting safety culture through sharing–a Dow perspective. **M.E. Jones**, L. Seiler, C. Mapes

8:55 CINF 32. Chemical and laboratory safety – the role of scholarly publishers. **C. Toro**, S.B. Tegen

9:20 CINF 33. Chemical safety data in the Handbook of Chemistry and Physics. **J. Rumble**, D.R. Lide, F. Macdonald

9:45 CINF 34. Safety sharing culture: Learning from the aviation industry. **T. Zoeller**

10:10 Intermission.

10:25 CINF 35. Information/practice sharing forums among American Chemistry Council member companies. **I. McGee**, D. Sandidge

10:50 CINF 36. Experiences with learning experience reports. **W.B. Tolman**

11:15 CINF 37. Balancing act: Protecting all interests. **S. Addlestone**, S. Christman

11:40 CINF 38. Parsing the "lessons learned" space: Layers of opportunities and challenges. **R. Stuart**

11:50 Panel Discussion.

Section B
New Orleans Marriott Convention Center
Natzhez

Workflows & Cheminformatics

R.J. Bienstock, G. Landrum, *Organizers, Presiding*

8:30 CINF 39. Open-source web tools for modeling and design tracking: Workflows facilitating collaborative drug discovery. **K.W. Lexa**, J.A. Feng

8:50 CINF 40. Building upon chemical similarity–methods to extend instance-based learning in cheminformatics. **T.H. Luechtefeld**

9:10 CINF 41. Chemical workflows supporting automated research data collection. **V. Tkachenko**, R. Zakharov, F. Prior, A.V. Kabanov, A. Tropsha

9:30 Intermission.

9:40 CINF 42. Diamond, XChem and CCP-CompMedChem: Creating user-focused tools and workflows for structure-based drug design. **A. Bradley**, R. Skyner, F. von Delft

10:00 CINF 43. How can you access PubChem programmatically? **S. Kim**, P. Thiessen, T. Cheng, E. Bolton

10:20 CINF 44. Interactive and reproducible data analysis with the open-source KNIME Analytics Platform. **G. Landrum**

10:40 Intermission.

10:50 CINF 45. Using Python to streamline access to the Cambridge Structural Database through new workflows. **P. Sanschagrin**, S. Vyas

11:10 CINF 46. Floe: Parallel, heterogeneous workflows on the cloud. **P.C. Hawkins**, A.G. Shewmaker, J.W. LaFon, A.G. Skillman, R.W. Tolbert

11:30 CINF 47. LiveDesign: Integrative molecular modeling and cheminformatics for collaborative drug design. **E. Davis**, T. Garland

Computational Catalyst Design for Energy Conversion & Storage

Advances in Theory, Computational Models & Approaches

Sponsored by COMP, Cosponsored by CATL and CINF

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Drug Design

QSAR & Docking

Sponsored by COMP, Cosponsored by CINF

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Applied Machine Learning: Molecular Dynamics, Materials & Virtual Screening

Sponsored by COMP, Cosponsored by CINF and PHYS

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
River Bend 1

Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web
Cosponsored by HIST and PRES
Financially supported by Clarivate Analytics
H.A. Lawlor, W.A. Warr, *Organizers*
M. Qiu, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 CINF 48. Eugene Garfield: The man and his legacy. **H.A. Lawlor**

1:50 CINF 49. From the Index Chemicus Registry System to SciFinder and beyond. **W.A. Warr**

‡*Cooperative Cosponsorship*

2:20 CINF 50. Eugene Garfield: The father of chemical text mining and artificial intelligence (AI) in cheminformatics. **R.A. Sayle**

2:50 Intermission.

3:00 CINF 51. Eugene Garfield's legacy and its impact on the culture of research. **S. Baykoucheva**

3:30 CINF 52. Beyond citations: What are new ways to assess content that will extend the assessment toolbox? **T.A. Carpenter**

4:00 CINF 53. Novel research and its scientific and technological impact. **J. Wang**

4:30 CINF 54. Clarivate Analytics: Building on the Garfield Legacy with web of science. **J. Testa**

5:00 Concluding Remarks.

Section B
New Orleans Marriott Convention Center
Natzhez

Workflows & Cheminformatics

R.J. Bienstock, G. Landrum, *Organizers, Presiding*

1:30 CINF 55. Quality data to quality models. **T. Hesketh**, P. Hunt, M.D. Segall, E. Champness, T. Mansley

1:50 CINF 56. Development and implementation of Amgen Small Molecule Projects Spotfire Report (ASMPSR) to streamline Hit2Lead and lead optimization process. **L. Jia**, S. Geuns-Meyer, H. Gao, T.G. Hopper, M. Southern, B. Lanman, Y. Sun

2:10 Intermission.

2:20 CINF 57. Automating matched molecular pair analysis of bioactivity and solubility data. **F. van den Broek**, M. Clark

2:40 CINF 58. Reaction and chemistry data blending. **M. Fischer**, J. Buckley, **F. van den Broek**

3:00 CINF 59. Integrated life science data and the power of workflows. J. Gurinova, D. Digles, **G.F. Ecker**

3:20 Intermission.

3:30 CINF 60. Automated workflows for data curation and standardization of chemical structures for QSAR modeling. **K. Mansouri**, A. McEachran, C. Grulke, A. Richard, R. Judson, A.J. Williams

3:50 CINF 61. Integrated visualization of the research landscape of proteins. **J. Gurinova**, G.F. Ecker

Computational Catalyst Design for Energy Conversion & Storage

Development of Electro- & Photocatalysts

Sponsored by COMP, Cosponsored by CATL and CINF

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Drug Design

Molecular Property

Sponsored by COMP, Cosponsored by CINF

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Deep Learning for Deep Chemical Understanding

Sponsored by COMP, Cosponsored by CINF and PHYS

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
E. Alvaro, *Organizer*

8:00–10:00

CINF 62. Analysis of food pairings based on food metabolites. **R. Reed**, T. Neumann

CINF 63. Interaction between organic phosphate ester and p53: An integrated experimental and *in silico* approach. **F. Li**

CINF 64. Teaching chemical information literacy: A 21st-century skill using 21st-century tools. **C. Hoffner**

CINF 65. Structure-based drug design for the zinc-dependent deubiquitinase STAMBPL1. S. Wussow, **C. Jaeger**, M. Buchholz

CINF 66. Triangulation of repurposing candidates for orphan diseases. **J. Gurinova**, D. Digles, G.F. Ecker

CINF 67. BioTransformer: A tool for metabolism prediction of small molecules. **Y. Djoumbou Feunang**, D. Wishart

CINF 68. Organizing the pathways and products of nerolidyl diphosphate into a searchable database. **R. Patnayakuni**, C. Hamann

CINF 69. Designing CDK2 inhibitors using the molecular chimera approach. **B. Cook**, D. Fourches

CINF 70. D-Peptide Builder: A web-based application to enumerate the chemical space of peptides. **B. Díaz Eufracio**, J.L. Medina-Franco, O. Palomino-Hernández

CINF 71. *De-novo* drug design with deep reinforcement learning. **M. Popova**, O. Isayev, A. Tropsha

CINF 72. One-click QSAR: A universal approach for developing accurate models. **V.M. Alves**, A. Golbraikh, E. Muratov, S. Capuzzi, K. Liu, W. Lam, D. Pozefsky, C.H. Andrade, A. Tropsha

TUESDAY MORNING

Section A
New Orleans Marriott Convention Center
River Bend 1

Chemical Information Literacy: Innovation, Collaboration & Assessment
Cosponsored by CHED
Y. Li, C. Lovitt, G.V. Szymczak, T.M. Vogel, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 CINF 73. Strategic outreach into chemistry and chemical engineering research groups at UC Berkeley. **K.K. Rupp**

9:00 CINF 74. Catalyzing chemical information literacy through ChemOnCampus. **D. Christe**

9:20 CINF 75. Creating bonds across campus: A general chemistry information literacy initiative. **D. Behmke**, **A. Harmer**

9:40 CINF 76. Helping users RAMP up by learning about chemical safety information resources. **G. Baysinger**

10:00 Intermission.

10:20 CINF 77. Using SurveyMonkey and Qualtrics to assess student learning in information literacy programs for undergraduate and graduate chemistry courses. **S. Baykoucheva**, A.J. Schech, E.C. Griffith

10:40 CINF 78. Building new information literacy collaborations at MTSU between library faculty and chemistry faculty. J.M. Iriarte-Gross, **M. Sloane**, D. Fitzgerald-Quintel, H. Listhartke, C. Groves

11:00 CINF 79. Continuous evolution of delivering chemical information literacy through the stepping stone approach. **A.A. Yeagley**, M.C. Rhoten, S.E. Porter, B. Topham

11:20 CINF 80. Building competency: Scaffolding information literacy skills throughout the chemistry curriculum. **C. Cowden**

11:40 Concluding Remarks.

Section B
New Orleans Marriott Convention Center
Natzhez

Cheminformatics Resources & Software Tools Supporting Environmental Chemistry
Cosponsored by COMP and ENVR
G. Patlewicz, A.J. Williams, *Organizers, Presiding*

8:30 CINF 81. Predictive computational techniques for chemical risk assessment. **D. Fourches**

8:50 CINF 82. Identifying and prioritizing chemicals for evaluation of potential endocrine bioactivity and exposure. **A. Frame**, K. Markey, A.S. Kamel, S. Watford, K. Paul-Friedman, R. Judson, A.J. Williams

9:10 CINF 83. OPERA: A free and open source QSAR tool for predicting physicochemical properties and environmental fate endpoints. **K. Mansouri**, C. Grulke, R. Judson, A.J. Williams

9:30 CINF 84. WebTEST (Web-services Toxicity Estimation Software Tool). **T. Martin**, V. Tkachenko, A.J. Williams

9:50 CINF 85. Literature-based cheminformatics for research in chemical toxicity. **N. Baker**, T. Knudsen, A.J. Williams

10:10 Intermission.

10:30 CINF 86. Chemotype-enrichment workflow: A univariate analysis workflow for exploring chemical feature enrichments across EPA's ToxCast chemical-assay landscape. **R. Lougee**, A. Richard, C. Grulke

10:50 CINF 87. New developments in delivering public access to data from the National Center for Computational Toxicology at the EPA. **A.J. Williams**, C. Grulke, A. McEachran, G. Patlewicz, I. Shah, J. Wambaugh, R. Judson, A. Richard, J. Edwards

11:10 CINF 88. Actualizing research into practical tools: A case study of GenRA, a new read-across tool. **G. Helman**, G. Patlewicz, I. Shah

11:30 CINF 89. Use of 2D chemical structure and bioactivity profiles to generate chemical categories within an Adverse Outcome Pathway network. **M. Nelms**, S.W. Edwards

11:50 CINF 90. COSMOS DB and ChemoTyper: Public resources for managing, sharing and exploring toxicity data and chemical space. **J.F. Rathman**, C. Yang, C. Schwab, O. Sacher, A. Tarkhov, J. Marusczyk, T. Kleinoeder, A. Mostrag, B. Bienfait

Computational Catalyst Design for Energy Conversion & Storage

Development of Homogeneous & Heterogeneous Catalysts

Sponsored by COMP, Cosponsored by CATL and CINF

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Jürgen Bajorath
Sponsored by COMP, Cosponsored by CINF and MEDI

TUESDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
River Bend 1

Chemical Information Literacy: Innovation, Collaboration & Assessment
Cosponsored by CHED
Y. Li, C. Lovitt, G.V. Szymczak, T.M. Vogel,

‡*Cooperative Cosponsorship*

Organizers, Presiding

1:30 Introductory Remarks.

1:35 CINF 91. Importance of synthetic speech mark-up language in the teaching of chemistry concepts in a multi-sensory way. **C.A. Supalo**, A.E. Neybert

1:55 CINF 92. Introducing cheminformatics early–prepares your students for success. **M. Pozenel**

2:15 CINF 93. What can you teach using PubChem? **S. Kim**, E. Bolton

2:35 CINF 94. Reaxys and you: Working together to prepare future chemists. **N. Xiao**, J. Swienty-Busch

2:55 Intermission.

3:15 CINF 95. Innovative instruction program for materials science and engineering undergraduate students. **S.J. Redalje**

3:35 CINF 96. Evolution of natural product total synthesis: Mapping pathways through literature searching. **L. McEwen**

3:55 CINF 97. Instructional scaffolding of information literacy skills in a problem-based learning context. **Y. Li**, **G.V. Szymczak**

4:15 CINF 98. Teaching information literacy through the chemistry laboratory. **C.E. Flener-Lovitt**, B. Finley, **A. Berger**

4:35 Discussion.
4:55 Concluding Remarks.

Section B
New Orleans Marriott Convention Center
Natzhez

Cheminformatics Resources & Software Tools Supporting Environmental Chemistry
Cosponsored by COMP and ENVR
G. Patlewicz, A.J. Williams, *Organizers, Presiding*

1:30 CINF 99. Machine learning methods for chemical properties and toxicity-based endpoints prediction using open-source libraries. **V. Tkachenko**, A. Korotcov, R. Zakharov, B. Sattarov, A. Mitrofanov

1:50 CINF 100. Exploring chemical space using *ChemMaps.com*. **A. Borrel**, N. Kleinstreuer, D. Fourches

2:10 CINF 101. Enhancing exchange of environmental data between EPA and FDA. **Y. Borodina**, S. Winfield, B. Pruitt

2:30 CINF 102. Prediction of pKa from chemical structure using free and open-source tools. **V. Tkachenko**, N. Cariello, A. Korotcov, K. Mansouri, A.J. Williams

2:50 CINF 103. Cheminformatics tools for supporting environmental chemistry. **Y. Djoumbou Feunang**, D. Wishart

3:10 Intermission.

3:30 CINF 104. Investigating ligand and structure-based modeling followed by mixture toxicity prediction of per-and polyfluoroalkyl substances: A virtual screening approach. **S. Kar**, S. Ghosh, J.R. Leszczynski

3:50 CINF 105. Chemoinformatic approach to identification of antiviral components in humic substances. **A. Orlov**, A.Y. Zherebker, A.A. Eletskaya, V.S. Chernikov, L.I. Kozlovskaya, Y.V. Zhernov, V.A. Palyulin, D.I. Osolodkin, I.V. Perminova

4:10 CINF 106. Adding complex expert knowledge into chemical databases: Transforming surfactants in wastewater. **E. Schymanski**, C. Grulke, J. Hollender, A.J. Williams

4:30 CINF 107. Prioritizing anthropogenic chemicals in drinking water sources through combined use of mass spectrometry based exposure data and ToxCast toxicity data. **A.M. Brunner**, M.M. Dingemans, K.A. Baken, A.P. van Wezel

Computational Catalyst Design for Energy Conversion & Storage

Development of Homogeneous & Heterogeneous Catalysts

Sponsored by COMP, Cosponsored by CATL and CINF

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Jürgen Bajorath
Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY MORNING

Section A
New Orleans Marriott Convention Center
River Bend 1

General Papers

E. Alvaro, *Organizer, Presiding*

8:30 CINF 108. Units of Measure Interoperability Service (UMIS): FAIR units for FAIR data. **S.J. Chalk**, R.J. Hanisch

8:55 CINF 109. RA21: Improving access to scholarly resources, from anywhere, on any device. **R. Youngen**

9:20 CINF 110. Rapid collection of experimental physicochemical property data to inform various models and testing methods. **C.I. Nicolas**, K. Mansouri, K. Phillips, C. Grulke, A. Richard, A. Williams, J. Rabinowitz, K. Isaacs, A. Yau, J. Wambaugh

9:45 Intermission.

10:00 CINF 111. Prediction of emission and absorption spectra for Eu^{2+}-doped inorganic phosphors based on stoichiometric information. **H. Nakano**, K. Tanaka, T. Miyao, K. Funatsu, R. Shirasawa, S. Tomiya

10:25 CINF 112. Deep learning approach to computational chemistry of lanthanides. **V. Tkachenko**, A. Mitrofanov, P. Matveev, A. Korotcov, R. Zakharov

10:50 CINF 113. Mapping of antiviral chemical space with ViralChEMBL: Use cases and new findings. **D.I. Osolodkin**, A. Orlov, A. Nikitina, L.I. Kozlovskaya, V.A. Palyulin, D. Horvath, A. Varnek

Drug Design

Algorithm, Tool & Web Service

Sponsored by COMP, Cosponsored by CINF

Structure-Based Drug Design for GPCRs
Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY AFTERNOON

Drug Design

Molecular Dynamics

Sponsored by COMP, Cosponsored by CINF

Structure-Based Drug Design for GPCRs
Sponsored by COMP, Cosponsored by CINF and MEDI

THURSDAY MORNING

Drug Design

Agonist, Antagonist & Macrocycle

Sponsored by COMP, Cosponsored by CINF

CHAL

Division of Chemistry and the Law

K. Bianco and J. Kennedy, *Program Chairs*

SOCIAL EVENTS:

Reception, 6:30 PM: Mon

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 213

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

A.H. Berks, *Organizer*
X. Pillai, *Organizer, Presiding*

2:00 CHAL 1. Review of recent Federal Circuit decisions relevant to what scientists need to know about patent filing and prosecution. **X. Pillai**, **A. Berks**

Legal Issues for Chemical Companies in the Food, Energy & Water Industries
Sponsored by SCHB, Cosponsored by CHAL and PROF

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 213

Issues in Chemical Commercialization
Cosponsored by BMGT
K.E. Bianco, *Organizer*
I. Hantman, *Organizer, Presiding*

9:30 CHAL 2. Issues in chemical commercialization. **K.E. Bianco**, **I. Hantman**, **G. Sower**

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 213

Update on Patent Eligibility: Are Things Getting Better for Patent Applicants?

J.L. Kennedy, *Organizer, Presiding*

1:30 CHAL 3. *Mayo, Alice, Prometheus, Enfish*? What is the current test for determining if an invention is eligible for patent filing? **R. Bone**, **J.L. Kennedy**

1:45 CHAL 4. How to patent medical diagnostics and genetics related inventions – What have recent cases taught us? **J.L. Kennedy**

2:30 CHAL 5. How to patent systems, software, and business method inventions – What have recent cases taught us? **R. Bone**

3:15 Discussion.

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix

K.E. Bianco, *Organizer*

8:00–10:00

CHAL 6. Chocolate: Food of the gods. **H.M. Peters**, **S.B. Peters**

CHAL 7. National Inventors Hall of Fame. **H.M. Peters**, **S.B. Peters**

TUESDAY AFTERNOON

Evolving Chemical Hazard Evaluation Strategies to Address Compliance under the New Toxic Substances Control Act (TSCA)
Sponsored by ENVR, Cosponsored by CHAL and CHAS

WEDNESDAY MORNING

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Sponsored by CHAS, Cosponsored by AGFD, CHAL and SCHB

‡*Cooperative Cosponsorship*

WEDNESDAY AFTERNOON

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Sponsored by CHAS, Cosponsored by AGFD, CHAL and SCHB

COLL

Division of Colloid and Surface Chemistry

R. Nagarajan, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Assembly & Colloidal Interactions of Cellulose Nanocrystals (see *CELL*, Sun, Mon)

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski (see *GEOC*, Sun, Mon, Wed)

Nano in Food, Energy, & Water (see *MPPG*, Mon)

Polymer Colloids: Synthesis, Analysis, Modeling & Applications (see *POLY*, Sun, Mon, Tue, Wed)

Polymers with Complex Architecture: From Synthesis to Self-Assembly (see *PMSE*, Sun, Mon, Tue, Wed)

Understanding the Complexity of the Nano/Bio Interface with Experiments & Computations (see *PHYS*, Wed, Thu)

SOCIAL EVENTS:

Social Hour with Poster Session, 6:00 PM: Sun

COLL Luncheon, 12:15 PM: Tue

BUSINESS MEETINGS:

COLL Business Meeting (Open), 5:30 PM: Sun

COLL Program & Executive Committee Meeting, 4:00 PM: Sat

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 242

Nanoparticle Biomolecule Corona: From Fundamentals to Applications

W. Chan, M. Hadjidemetriou, K. Kostarelos, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COLL 1. Relevance of the biomolecule corona for nanomaterial-microbe cross-talk. **R. Stauber**, S. Knauer, D. Westmeier

9:05 COLL 2. Spontaneous lipid corona formation at lipid bilayers. **F. Geiger**

9:25 COLL 3. Interfacially-stabilized polymeric nanosystems for drug delivery. **M.A. Ilies**, U. Satyal, J.A. Shif, V.D. Sharma

9:45 COLL 4. Dynamic remodeling of synthetic lipoproteins in blood serum solutions. **S.F. Gilmore**, S. Peters, P.T. Henderson, C. Blanchette, N. Fischer

10:05 Intermission.

10:25 COLL 5. Mechanisms of binding and assembly of complement factors on nanoparticles. **D. Simberg**, F. Chen, G. Wang, S.M. Moghimi, V.P. Vu

10:55 COLL 6. Gold nanoparticles and proteins: Quid pro quo. **L. Liz Marzan**

11:25 COLL 7. Protein interactions with stealth-coated gold nanoparticles. **N.T. Flynn**, A.W. Cheema, A.L. Code, M.T. Phan, A. Uchitelle, A. Webb

11:45 COLL 8. Structure and orientation of a small protein on a gold nanoparticle surface. **Y.R. Perera**, A. Huges, N. Fitzkee

Section B
Ernest N. Morial Convention Center
Room 245

Biomaterials & Biointerfaces

Bacteria at Interfaces in the Environment

A.P. Goodwin, *Organizer*
V. Gordon, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 COLL 9. Using an environmentally-relevant panel of Gram-negative bacteria to assess the toxicity of polyelectrolyte-wrapped gold nanoparticles. **J.T. Buchman**, A. Rahnamoun, K.M. Landy, X. Zhang, A. Vartanian, L. Jacob, C.J. Murphy, R. Hernandez, C.L. Haynes

9:00 COLL 10. Force-modulated multivalent binding of fimbriated bacteria. **E. Reimhult**, A. Lundgren, P. van Oostrum

9:20 COLL 11. Clay-based microstructures as alternatives to chemical dispersants in bioremediation of crude oil: Studies with model marine organisms. **L.T. Swientoniewski**, M. Omarova, R. Blake, T. Yu, S. Zhang, A. Panchal, Y.M. Lvov, D. Zhang, V.T. John, D.A. Blake

9:40 COLL 12. Remodeling of fluid interfaces by bacteria. **D. Lee**, T.H. Niepa, L. Vaccari, R. Leheny, M. Goulian, K.J. Stebe

10:10 COLL 13. Structure and mechanics of microbial biofilms. **J. Wilking**

10:40 Intermission.

11:00 COLL 14. Programmable bacterial biofilms via growth microenvironments. **A. Hochbaum**

11:30 COLL 15. Bacterial interactions with immobilized liquid surfaces. **C. Howell**, J. Aizenberg

12:00 COLL 16. Understanding heterogeneous populations of *P. aeruginosa* at the single-cell level. **C. Chang**

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, M. Nieh, A.N. Parikh, *Organizers*
S. Muralidharan, *Organizer, Presiding*
C. Naumann, *Presiding*

8:30 COLL 17. Molecular dynamics simulation study of alpha-tocopherol interaction with lipid bilayers. **S. Kavousi**, B. Novak, D. Moldovan

8:50 COLL 18. Amphiphilic polypeptoids connect nanoparticle containing lipid rafts onto lipid membranes through self-assembly. **V.T. John**, Y. Zhang, T. Yu, M. Omarova, D. Zhang

9:20 COLL 19. Systematic study of structure-function relationships in synthetic, archaea-inspired tetraether lipids. G. Leriche, T. Koyanagi, Y. Kim, K. Gao, D. Onofrei, O. Eggenberger, N.C. Gianneschi, G.P. Holland, M.K. Gilson, D. Sept, M. Mayer, **J.C. Yang**

9:50 COLL 20. Interplay between passive and active membrane mechanisms regulates the formation of the immunological synapse. **O. Farago**

10:20 COLL 21. Ultra coarse-grained molecular dynamics simulations of lipid bilayers. J. Carrillo, J. Katsaras, **B. Sumpter**, R. Ashkar

10:50 COLL 22. Phonon-mediated biological functions of a cell membrane. **M. Zhernenkov**

11:20 COLL 23. Melting and exchange kinetics of nano-crystalline micelles: Implications for lipid dynamics. **R. Lund**, N. Koenig, T. Zinn, L. Willner

11:50 COLL 24. Withdrawn

Section D
Ernest N. Morial Convention Center
R06

Chemistry of Molecular Electronics

Theory

Cosponsored by PHYS
M.S. Inkpen, G.C. Solomon, L. Venkataraman, *Organizers, Presiding*

8:30 COLL 25. Two-dimensional pi-conjugated covalent organic networks: Establishing chemical structure – electronic properties relationships. **J.E. Bredas**

9:00 COLL 26. Computational tools for chemical insight in molecular electronics. **G.C. Solomon**

9:20 COLL 27. Charge transport mechanisms in molecular junctions. **D. Segal**

9:50 COLL 28. First-principles calculations of charge transport: Weakly coupled and strongly coupled molecular junctions. **Z. Liu**, S. Refaely-Abramson, F. Bruneval, J. Neaton

10:10 COLL 29. In search of structure-activity relationships in transition metal-based molecular conductors. **J. Mcgrady**, V. Arcisauskaite, J. Lamb

10:40 Intermission.

10:50 COLL 30. Quantum-interference-enhanced thermoelectricity in single-molecule junctions. **C.J. Lambert**

11:20 COLL 31. Utilizing the helical frontier orbitals of cumulenes in molecular electronics. **M.H. Garner**, R. Hoffmann, A. Jensen, L. Hyllested, S. Rettrup, G.C. Solomon

11:40 COLL 32. Spin-polarized transport through molecular junctions from first principles. **C. Herrmann**

12:00 COLL 33. Moving electrons: Quantum transport, time dependence, phonons, interference and probes. **M.A. Ratner**

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
M. Cai, H. Fan, Y. Han, *Organizers*
F. Bai, *Organizer, Presiding*
H. Fan, *Presiding*

8:30 COLL 34. Bimetallic Janus nanocrystals. **Y. Xia**

9:00 COLL 35. Crystal phase-engineering of novel nanomaterials. **H. Zhang**

9:30 COLL 36. Understanding the removal pathways of dislocations in imperfectly attached nanocrystals using *in-situ* HRTEM. **J. Ondry**, M.R. Hauwiller, P. Alivisatos

9:50 COLL 37. Controlled syntheses of gold nanostars for stronger surface enhanced Raman scattering. **C. Jiang**

10:10 Intermission.

10:30 COLL 38. Fluorescene kidney functional imaging enabled by renal clearable gold nanoparticles. **J. Zheng**, M. Yu

11:00 COLL 39. Do nucleation and growth have to be twin events in nanoparticle formation? **Y. Sun**

11:30 COLL 40. One-pot synthesis of heterostructured RuCu alloyed nanotubes. **H. Cheng**, H. Zhang

11:50 COLL 41. Understanding the mechanism of non-equilibrium etching of gold nanocrystals through graphene liquid cell TEM. **M.R. Hauwiller**, L.B. Frechette, M.R. Jones, J. Ondry, P.L. Geissler, P. Alivisatos

12:10 COLL 42. Chemical soldering of nanoparticle assemblies for photovoltaic applications. **N.N. Kholmicheva**, M. Zamkov

Section F
Ernest N. Morial Convention Center
R09

Fundamental Studies of Mechanochemical & Tribochemical Processes at Interfaces

R.M. Espinosa-Marzal, W.T. Tysoe, *Organizers*
J.D. Batteas, *Organizer, Presiding*

8:30 Introductory Remarks.

‡*Cooperative Cosponsorship*

8:35 COLL 43. Stress-assisted thermal activation in tribology: from friction and rheology to wear and tribo/mechanochemistry. **W.T. Tysoe**

9:05 COLL 44. First-principles modeling of the joint influences of catalysis and mechanical stress in tribopolymer formation. **A.M. Rappe**

9:35 COLL 45. Constituents of tribochemistry – molecule and surface at shearing interface: how would their chemical structure affect the critical activation volume of mechanochemical reaction? **S.H. Kim**

10:05 Intermission.

10:20 COLL 46. Mechanochemical synthesis, structure and properties of solid solutions of alkaline earth metal fluorides $M^a_xM^b_{1-x}F_2$ (M = Ca, Sr, Ba, Pb). **G. Scholz**

10:50 COLL 47. Emergence and applications of techniques for real-time monitoring of mechanochemical reactions. **T. Friscic**

11:20 COLL 48. Exploring pharmaceutical cocrystal diversity using liquid-assisted mechanocheical reactions. **W. Jones**

11:50 COLL 49. Dissipation pathways upon sliding a tip along the calcite-brine interface: Connection between nanotribology and mineral reactivity. **Y. Diao**, R.M. Espinosa-Marzal

Section G
Ernest N. Morial Convention Center
Room 203

Nanomaterials

Nanoscience in Industry & Manufacturing

J.A. Hollingsworth, *Organizer*
R. Nagarajan, *Organizer, Presiding*

8:30 COLL 50. Improving mechanical properties in glassy polymer nanocomposites: Effect of molecular weight. **V. Bocharova**, A. Genix, A. Kisliuk, S. Zhao, A.P. Sokolov

8:50 COLL 51. Functional nanomaterials: Towards magnetically activated adhesives. **G. Davies**

9:10 COLL 52. Developing quantum-dot nanocomposites for high-performance luminescent solar concentrators. **A. Jackson**, M. Bergren, N. Markarov, K. Ramasamy, H. McDaniel

9:30 COLL 53. Real-time, *in situ* observation of aqueous corrosion initiation in nanostructured steel. **S.C. Hayden**, C. Chisholm, R.O. Grudt, W. Mook, A. Ilgen, D. Bufford, K. Hattar, T.J. Kucharski, I. Taie, K. Jungjohann, M. Ostraat

9:50 COLL 54. Light, but strong SiC foam for thermal insulation and electromagnetic interference shielding at elevated temperatures. **Z. Wang**

10:10 COLL 55. Volumetric, percolating metallic structures templated by laser-deposited carbon nanofoams: Applications in humidity sensing. **S. Nufer**, J.P. Salvage, A. Shmeliov, A. Brunton, A. Dalton

10:30 COLL 56. Unusual ion-exchange behavior of nanoparticulate oxides: Applications in food, energy, and water sectors. **A.W. Apblett**, C.K. Perkins, T. Reed

10:50 COLL 57. Nanoaptasensors based on gold nanotriangles for the efficient and selective detection of ochratoxin A via LSPR and SERS. **Y. Hernandez**, L. Lagos, B.C. Galarreta

11:10 COLL 58. Preparation and toughening performance investigation of epoxy resins containing carbon nanotubes modified with hyperbranched polyester. **L. Lu**, X. Liao

Section H
Ernest N. Morial Convention Center
Room 204

Basic Research in Colloids, Surfactants & Nanomaterials

Nanoparticle Synthesis & Assembly

R. Nagarajan, *Organizer*
F. Bai, *Presiding*

8:30 COLL 59. Precursor ion–ion aggregation in the Brust–Schiffrin synthesis of alkanethiol nanoparticles. **T. Graham**, R. Renslow, N. Govind, S.R. Saunders

8:50 COLL 60. Synthesis and characterization anisotropic rod-like colloids with thermoreversible short-range attractions: Towards a universal phase diagram for adhesive hard rod suspensions. **N.J. Wagner**, R.P. Murphy

9:10 COLL 61. Understanding self-assembly and ionic strength interactions of cellulose nanocrystals using isothermal titration calorimetry and rheology. **E. Facchine**, S. Jin, R.J. Spontak, O.J. Rojas, S. Khan

9:30 COLL 62. Every which way but loose: A single thermoresponsive diblock copolymer can form spheres, worms or vesicles in aqueous solution. **S.P. Armes**

9:50 COLL 63. Synthesis of anisotropic nanostructures through controlled symmetry breaking. **A.E. Kossak**, B. Stephens, Y. Tian, P. Liu, M. Chen, T.J. Kempa

10:10 COLL 64. Controlled self-assembly of porphyrin and catalytic applications. **F. Bai**

10:30 COLL 65. Tuning local nanoparticle arrangements and dynamical properties in polymer nanocomposites by grafting of small molecules. **A. Genix**, D. Musino, V. Bocharova, A.P. Sokolov, J. Oberdisse

10:50 COLL 66. Spectroscopy nanosensors based on Zika virus Sn1 antibodies linked to gold nanoparticles: A system optimization study. **R.L. Silveira**, J. Santos, J. Rubim, P. Corio

11:10 COLL 67. Three-dimensional assemblies of $Fe_{2-x}Ni_xP$ ($0 \le x \le 2$) and $Co_{2-y}Fe_yP$ ($0 \le y \le 2$) nanoparticles and their magnetic properties: Towards effective magnetic refrigerant materials. **M.A. Hettiarachchi**, S. Brock, E. Abdelhamid, B. Nadgorny

11:30 COLL 68. Concentric Nd(III)-sensitized core-shell upconversion nanoparticles for excitation with biobenign wavelength. **C. Arboleda**, S. He, A. Stubelius, N. Johnson, A. Almutairi

Section I
Ernest N. Morial Convention Center
Room 205

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Atomic-Level Precision in Deposition & Etching

Cosponsored by WCC
A.V. Teplyakov, *Organizer*
H. Lee, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL 69. Withdrawn

9:05 COLL 70. Topographically selective atomic layer deposition on 3D nanostructures for novel nanopatterning processes. **W. Kim**, S.F. Bent

9:35 COLL 71. Surface reactions for area-selective atomic layer deposition and thermal atomic layer etching of metals and dielectrics. **G. Parsons**

10:05 COLL 72. Surface chemistry of metal atomic layer deposition (ALD) precursors. **F. Zaera**

10:35 Intermission.

10:50 COLL 73. A tale of two coordination modes: Diaminoalkylsilane adsorption on dielectric and silicon substrates. **J. Kachian**

11:20 COLL 74. Surface chemistry of thermal atomic layer etching. **S.M. George**

11:50 COLL 75. Withdrawn

Section J
Ernest N. Morial Convention Center
Room 225

Basic Research in Colloids, Surfactants & Nanomaterials

Surfactants

R. Nagarajan, *Organizer*
K. Sakurai, *Presiding*

8:30 COLL 76. Effect of micelle structure and inter-micellar interactions on multicomponent diffusion in nonionic micellar solutions. **N.P. Alexander**, S.R. Dungan, R. Phillips

8:50 COLL 77. Molecular dynamics investigation of ionic interfacial partitioning in reverse micelles. **A.K. Sharma**

9:10 COLL 78. Transitions between non-equilibrium micelles. **F. Plamper**, N. Warren, A. Steinschulte

9:30 COLL 79. Platonic micelles part 1: Monodispersity and discreteness of the aggregation number of calix[4] arene-based micelles bearing non-ionic hydrophilic groups. **S. Fujii**, R. Takahashi, K. Sakurai

9:50 COLL 80. Platonic micelles part 2: Thermodynamic and kinetic consideration of the micelles with the discrete aggregation numbers and mono-dispersity. **K. Sakurai**, R. Takahashi, S. Fujii

10:10 COLL 81. Structural and thermodynamic impact of diproplyne glycol (DPG) on mixed surfactant system. **H. Jiang**, K. Vogtt, G. Beaucage, M.R. Weaver

10:30 COLL 82. Intermolecular headgroup interaction and hydration as driving forces for lipid transmembrane asymmetry. N. Smolentsev, C. Luetgebaucks, H. Okur, **S. Roke**

10:50 COLL 83. Force mapping and characterization of surfactant adsorbed on flat and patterned surfaces. **J. Hamon**, B.P. Grady, R. Tabor, A. Striolo

11:10 COLL 84. Electrochemical diffusion coefficients for cationic surfactants using ferrocene probes. **S.J. Bachofer**, B. Schepergerdes, M.D. Lingwood

11:30 COLL 85. Transport properties in micelle nanoreactors: Molecular modeling approach. **C. Callaway**, S. Jang, K.R. Hendrickson, N. Bond, S. Lee

11:50 COLL 86. Studying the Interaction of Hydrophobically modified Ethoxylated URethane (HEUR) polymers with Sodium Dodecylsulfate (SDS) in aqueous solution. **M. Ibrahim**, P. Griffiths, M.W. Murray, A. Szczygiel

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms & Selectivity

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Physical Chemistry of Ionic Liquids

Functional Ionic Liquids & Applications

Sponsored by PHYS, Cosponsored by COLL‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

‡*Cooperative Cosponsorship*

Section A
Ernest N. Morial Convention Center
Room 242

Nanoparticle Biomolecule Corona: From Fundamentals to Applications

W. Chan, M. Hadjidemetriou, K. Kostarelos, *Organizers, Presiding*

2:00 COLL 87. Engineering protein coronas for applications in nanomedicine. **K. Hamad-Schifferli**

2:30 COLL 88. Biomolecular corona of gold nanoparticles formed in blood: Application for detection and diagnosis of infectious diseases and cancer. T. Zheng, **Q. Huo**

3:00 COLL 89. Nanoscale tools for biomarker discovery: The emerging role of biomolecule corona. **M. Hadjidemetriou**, K. Kostarelos

3:20 COLL 90. Protein coronas enhance polystyrene interactions with a model human erythrocyte membrane outer leaflet. **N. Ganji**, G.D. Bothun

3:40 Intermission.

4:00 COLL 91. Interaction of proteins with nanoparticles probed with non-optical methods. **W. Parak**

4:30 COLL 92. Selective blood vessel deletion using nanoparticle-mediated drug delivery in zebrafish embryos. **A. Kros**

5:00 COLL 93. Protein, lipid membrane and cell interactions of PEGylated and POZylated superparamagnetic iron oxide nanoparticles. **E. Reimhult**, A. Lassenberger, N. Gal, S. Kurzhals, E. Benetti, R. Zirbs

5:20 COLL 94. Suppressing nanoparticle-mononuclear phagocyte system interactions of two-dimensional gold nanorings for improved tumor accumulation and photothermal ablation of tumor. **Y. Liu**, Z. Nie, X. Chen

5:40 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 245

Biomaterials & Biointerfaces

Bacteria at Interfaces in Healthcare

A.P. Goodwin, *Organizer*
V. Gordon, *Organizer, Presiding*

2:00 COLL 95. Glycan engineering at nanoparticle surfaces to understand and detect infection. B. Martyn, S. Won, S. Richards, **M.I. Gibson**

2:20 COLL 96. Bacterial display of peptides for control of bacteria-gold interfaces. **D.A. Sarkes**, J.J. Rice, H. Dong, J. Terrell, J.P. Jahnke, M.C. Small, M. Hurley, D.N. Stratis-Cullum

2:40 COLL 97. Biological colloids: Bacterial outer membrane vesicles. E.S. Rasti, J.B. Nice, **A.C. Brown**

3:00 COLL 98. Adhesion and viscoelasticity of living tissues: The Live Cell Monolayer Rheometer (LCMR). **G.G. Fuller**, J. Pokki, M. Merola, A. Undieh, E. Hollenbeck, L. Cegelski

3:30 COLL 99. Shake it off: Dynamics of bacterial adhesion at interfaces. S. Sharma, Y.A. Jaimes-Lizcano, V. Yadav, R.B. McLay, P. Cirino, M.L. Robertson, **J. Conrad**

4:00 Intermission.

4:20 COLL 100. Mechanical and chemical properties of polymer hydrogels influence bacterial adhesion. K.W. Kolewe, **J.D. Schiffman**

4:50 COLL 101. How bacteria sense surfaces to begin biofilm development, and how we might thwart surface sensing to prevent biofilm development. **V. Gordon**

5:10 COLL 102. Transparent copper-containing coatings for inhibiting bacterial transmission. **K. Neoh**, D. Mitra, E. Kang

5:30 COLL 103. Interaction of bacterial cells with model graphene oxide surfaces: Insights from single-cell force spectroscopy. **S. Romero-Vargas Castrillon**

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A.N. Parikh, *Organizers*
M.L. Longo, A.B. Subramaniam, *Presiding*

2:00 COLL 104. Preparation and characterization of nanopore supported phospholipid bilayers for Raman microscopy detection and quantification of membrane-associated signaling peptides. **D. Bryce**, J.P. Kitt, J.M. Harris

2:20 COLL 105. Quantifying the electrostatics of polycation–lipid bilayer interactions. **F. Geiger**

2:50 COLL 106. Exploring cellular mechanosensitivity using cell surface-mimicking substrates. **C. Naumann**, K. Shilts

3:20 COLL 107. Charge switch regulating structures and dynamics of lipid membrane. **M. Choi**

3:50 COLL 108. Smart polymersomes as structural analogues of eukaryotic cells: From membrane asymmetry to compartmentalization. A. Peyret, L. Beaute, E. Ibarboure, O. Sandre, J. Le Meins, N.D. McClenaghan, **S. Lecommandoux**

4:20 COLL 109. Coupling of lipid membrane elasticity and dynamics. **Y. Chen**

4:50 COLL 110. Antioxidant implication of the physical presence of vitamin E in lipid membranes. M. DiPasquale, M. Nguyen, **D. Marquardt**

Section D
Ernest N. Morial Convention Center
R06

Chemistry of Molecular Electronics

Molecular-Scale Electronics

Cosponsored by PHYS
M.S. Inkpen, G.C. Solomon, L. Venkataraman, *Organizers, Presiding*

2:00 COLL 111. Enhancing the thermoelectric properties of molecular junctions. **N. Agrait**

2:30 COLL 112. Gating of junction conductance by charge transfer complex formation in single molecule devices. A. Vezzoli, K. Wang, I. Grace, R. Nichols, C.J. Lambert, B. Xu, **S.J. Higgins**

2:50 COLL 113. Quantum interference effects in the charge transport through single-molecule junctions. **W. Hong**

3:20 Intermission.

3:30 COLL 114. Metal complexes for molecular electronics and Moore. **P.J. Low**

4:00 COLL 115. Reduced length-dependent conductance decay in polymethine molecular wires. **S. Gunasekaran**, I. Davydenko, D. Hernangomez-Perez, F. Evers, S.R. Marder, L. Venkataraman

4:20 COLL 116. Room-temperature current blockade in atomically defined single-cluster junctions. **X. Roy**, L. Venkataraman, B. Choi, G. Lovat

4:50 COLL 117. Dual control of chemical equilibria through pH and potential in single-molecule devices. R. Brooke, D. Szumski, A. Vezzoli, S.J. Higgins, R. Nichols, **W. Schwarzacher**

5:10 COLL 118. Mechanical stretching-induced electron transfer reactions and conductance switching in single molecules. **N. Tao**, Y. Li, N. Haworth, L. Xiang, S. Ciampi, M. Coote

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
M. Cai, H. Fan, Y. Han, *Organizers*
F. Bai, *Organizer, Presiding*
H. Fan, *Presiding*

2:00 COLL 119. Design and assembly of coupled multicomponent nanocrystal superlattices and quasicrystalline assemblies and superparticles. **C.B. Murray**, Y. Wu, Z. Li, K. Elbert, D. Jishkariani, M. Zhang, C.R. Kagan, S. Najmr, D. Wang

2:30 COLL 120. Large-scale assembly of 2-D honeycomb semiconductor superlattices and their incorporation in opto-electronic devices. **D. Vanmaekelbergh**, J. Peters, S. Buhbut-Sinai, M. Alimoradi Jazi, G. Soligno, J. Geuchies

3:00 COLL 121. *In situ* space- and time-resolved small angle x-ray scattering to probe electric field-driven assembly of nanocrystal superlattices. **Y. Yu**, C. Orme

3:20 Intermission.

3:30 COLL 122. Nanomanufacturing by self-assembly. **N. Kotov**

4:00 COLL 123. *In-situ* scattering techniques to study synthesis and crystallization processes of colloidal nanocrystals. **M. Cargnello**, L. Wu, J. Qin, C. Tassone

4:30 COLL 124. Tracking micelle growth during polymerization-induced self-assembly with liquid cell transmission electron microscopy. **M.A. Touve**, C.A. Figg, D. Wright, C. Park, J. Cantlon, B.S. Sumerlin, N.C. Gianneschi

4:50 COLL 125. Improved synthetic efficiency and greener preparation of gold nanorods. **J.W. Stone**

5:10 COLL 126. Utilization of colloidal plasmonic metal nanoparticles for understanding polymer chemistry. **G. Liu**

Section F
Ernest N. Morial Convention Center
R09

Fundamental Studies of Mechanochemical & Tribochemical Processes at Interfaces

J.D. Batteas, R.M. Espinosa-Marzal, *Organizers*
W.T. Tysoe, *Organizer, Presiding*

2:00 COLL 127. Tribochemical nanolithography. **G.J. Leggett**

2:30 COLL 128. Interrogating force-induced reaction acceleration on bond-forming surface reactions. **A.B. Braunschweig**

3:00 COLL 129. Chemistry of trinuclear molybdenum compounds and impact on friction. A. Jaishankar, A. Konicek, A. Jusufi, **A.M. Schilowitz**

3:20 COLL 130. Dynamic motion and energy dissipation in graphene on rough surfaces. **M.B. Elinski**, J. Batteas

3:40 Intermission.

3:55 COLL 131. Chemistry of friction, wear, and tribofilm growth on 2D materials. S. Raghuraman, M. Elinski, J. Batteas, **J.R. Felts**

4:25 COLL 132. Probing the load/strain dependent reaction of Perfluorophenylazide (PFPA) with graphene. **J.D. Batteas**, M.B. Elinski, M. Negrito

4:45 COLL 133. High throughput and multi-scale quantum-mechanics / molecular-mechanics calculations applied to lubricants. **M. Righi**, P. Restuccia, G. Fatti

5:15 COLL 134. Thermodynamic basis of friction in MoS_2. **M. Chandross**, A. Hinkle, T. Babuska, J. Curry, B. Krick, M. Dugger, N. Argibay

Section G
Ernest N. Morial Convention Center
Room 203

Nanomaterials

Surface Chemistry & Modification

J.A. Hollingsworth, R. Nagarajan, *Organizers*
M.A. Firestone, *Presiding*

2:00 COLL 135. Facile surface exchanges in CdSe quantum belts. **W.E. Buhro**, Y. Yao, Y. Zhou

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2:30 COLL 136. Quantum dot-ligand equilibrium in purified samples. **A.B. Greytak**

3:00 COLL 137. Consequences of InP quantum dot modification using fluoride. **E.J. McLaurin**, R. Siramdas, M. Yazdanparast, S. Lee, C. Aparicio, J.M. Rosado

3:30 COLL 138. Orthogonal chemical modification of template-synthesized nanostructures with oligonucleotides. **T. Oh**, J. Park, J.C. Ku, T. Ozel, C.A. Mirkin

3:50 COLL 139. Modeling nanomaterial properties: Effects of surface chemistry and interfacial couplings. P.A. Brown, E.I. Calixte, O.N. Samoylova, **K.L. Shuford**

4:10 COLL 140. Approach to retard oxidation during processing of colloidal Ti_3C_2 MXenes. **T. Habib**, S. Shah, W. Sun, E. Prehn, Z. Tan, M.J. Green, M. Radovic

4:30 COLL 141. Investigation of charge-based chromatographic methods for sorting carbon nanotube chiral forms. **P. Rezaei**, D. Frey, L.D. Pfefferle

4:50 COLL 142. nano-FTIR: Infrared imaging and spectroscopy with 20nm spatial resolution. **T. Gokus**, P. Schäfer

5:10 COLL 143. Binding of hydrogen and phenol at a Pt_{50} nanoparticle supported on graphene: *Ab initio* molecular dynamics simulations. **M. Nguyen**, D.C. Cantu, V. Glezakou, R. Rousseau

Section H
Ernest N. Morial Convention Center
Room 204

Surface Chemistry

Nanoparticle & Liquid Surfaces

S.L. Tait, *Organizer*
A.L. Mifflin, L. Seballos, *Presiding*

2:00 COLL 144. Ligand ordering phase transitions in mixed ligand shells of CdSe/CdS quantum dots. **A. Balan**, J.H. Olshansky, P. Alivisatos

2:20 COLL 145. Role of ligand interactions in CdSe quantum dot ligand exchange dynamics. **E. O'Brien**, P. Alivisatos

2:40 COLL 146. Investigating molecular interactions on silver nanostructures using density functional theory and surface-enhanced Raman scattering. **L. Seballos**

3:10 COLL 147. Absolute, complex spectral measurement: Turning SFG (sum frequency generation) into an analytical technique. **M.J. Shultz**, P.J. Bisson, J.M. Marmolejos, J. Wang

3:40 COLL 148. Fabrication of micro- and nano-sized metal structures on silicon and mica substrates: An Atomic Force Microscope (AFM) and Particle Lithography (PL) approach. **S.B. Ulapane**, A.K. Borkowski, M.K. Okeowo, J. Totleben, C.L. Berrie

4:00 COLL 149. Direct optical lithography of functional inorganic nanomaterials. **Y. Wang**, I. Fedin, H. Zhang, D. Talapin

4:20 COLL 150. Adsorption of water on kaolinite and montmorillonite surfaces, and its effect on CO_2 adsorption: DFT calculations. R.A. Bennick, M.D. Kilmer, **L. Tribe**

4:50 COLL 151. Surface interactions of the siderophore desferrioxamine-B with hematite/water interfaces studied using second harmonic and sum frequency generation spectroscopies. **A.L. Mifflin**

5:20 COLL 152. Jones-Ray effect reinterpreted: Surface tension minima of low ionic strength electrolyte solutions are caused by electric field induced water-water correlations. H. Okur, Y. Chen, D. Wilkins, **S. Roke**

Section I
Ernest N. Morial Convention Center
Room 205

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Nanomaterials & Catalysis on the Nanoscale

Cosponsored by WCC
H. Lee, *Organizer*
A.V. Teplyakov, *Organizer, Presiding*

2:00 COLL 153. Relative stabilities of reaction intermediates on group 1B metals: Effects of van der Waals interactions and bonding structure. **R.J. Madix**

2:30 COLL 154. Infrared spectroscopy of the water gas shift reaction over the Cu(111) surface under ambient pressure conditions. C. Kruppe, **M. Trenary**

3:00 COLL 155. Accelerated discovery of materials for solar thermal water splitting using computational chemistry and machine learning. **C. Musgrave**, S. Millican, R. Trottier, C. Bartel

3:30 COLL 156. Photoelectochemical and electrochemical fuel production using low dimensional catalytic materials. **U. Sim**

4:00 Intermission.

4:15 COLL 157. Photocatalysis at diamond surfaces: New approaches to photochemical reduction reactions. **R.J. Hamers**

4:45 COLL 158. Translation of fundamental studies of surface chemistry to catalytic function in nanoporous materials. **C.M. Friend**

5:15 COLL 159. Nanoparticle catalysis: Understanding the role of the surface and surface-passivation in creating stable, efficient and scalable devices. **S. Geyer**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski
Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms at the Atomic Scale

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Assembly & Colloidal Interactions of Cellulose Nanocrystals
Sponsored by CELL, Cosponsored by COLL

Physical Chemistry of Ionic Liquids

Functional Ionic Liquids & Applications

Sponsored by PHYS, Cosponsored by COLL‡

Magnetically Recoverable Catalysts
Sponsored by CATL, Cosponsored by COLL, ENFL and INOR

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls B2/C

Fundamental Research in Colloids, Surfaces & Nanomaterials

R. Nagarajan, *Organizer*

6:00–8:00

COLL 160. Interparticle hydrogen bonding influences the shear jamming of dense colloidal suspensions. **N. James**, E. Han, R. Lopez de la Crus, H. Jaeger

COLL 161. Sensor made of graphene oxide and upconversion nanoparticles to sense mRNA biomarkers. D. Giust, M. Lucio-Benito, O. Muskens, **A. Kanaras**

COLL 162. Determination of interfacial amorphicity in functional powders. M. Badal Tejedor, **N. Nordgren**, M. Schuleit, S. Pazesh, G. Alderborn, A. Millqvist-Fureby, M.W. Rutland

COLL 163. Understanding the galinstan oxide interface through interfacial tension and interfacial rheology for use in stretchable applications. **A. Koh**, R. Mrozek, G. Slipher

COLL 164. Quantitative analysis of temperature programmed desorption from complex surfaces: A machine learning approach to surface science. **A.C. Elder**, T.M. Orlando

COLL 165. Adsorption of water and gaseous species on calcite surfaces at different relative humidity and temperature. **N.A. Wojas**, A. Swerin, P. Claesson, V. Wallqvist, M. Järn, P. Gane, J. Schoelkopf, M. Adam

COLL 166. Morphological transformations from supramolecular nanofibers to nanoribbons in self-assembly of conjugated block copolymers. **M. Wang**, L. Han, F. He

COLL 167. Super liquid repellent surfaces – non-wetting forces, cavity growth and coatings on biobased materials. **A. Swerin**

COLL 168. Eliminating intracellular *S. aureus* with its nanoparticle mimetic. F. Gao, L. Xu, **L. Yang**

COLL 169. High efficacious nanoemulsion (NE) formulation of polyunsaturated fatty acid-taxoid conjugates. **Y. Zhang**, C. Wang, G. Ahmad, M. Amiji, J. Rooney, T. Zimmerman, I. Ojima

COLL 170. Single-molecule fluorescence sheds light on coupled dye-nanoparticle systems. **T. Zuo**

COLL 171. Electrochemically enhanced dissolution of silica and alumina in alkaline environments. **H.A. Dobbs**, K. Kristiansen, A.M. Schrader, Z. Berkson, G. Degen, B. Chmelka, J.N. Israelachvili

COLL 172. Towards Polarization-Switched Solid-State Molecular (POSSM) pumps. **C. Fernandez**, E. Polikarpov, G. Coffey, A.J. Karkamkar, S.K. Nune, P. Koech, W. Xu, P. McGrail

COLL 173. Optically transparent ultramicroelectrode for studying local electrochemical events of single Au nanoparticle using combined methods of electrochemistry and dark field scattering microscopy. **Y. Ma**, A. Highsmith, S. Pan

COLL 174. Electronic transport in supromolecular peptide nanofibers. **A. Hochbaum**, N. Ing, R.K. Spencer

COLL 175. Understanding the anticorrosive protective mechanisms of modified epoxy coatings with combined improved barrier, active feedback, self-healing and antimicrobial functionalities using advanced electrochemical and spectroscopic techniques. **D.I. Njoku**, M.M. Cui, H. Xiao, B. Shang, Y. Li

COLL 176. Withdrawn

COLL 177. 2D materials grafted colloidal microparticles. **A.T. Liu**, P. Liu, M. Strano

COLL 178. Controllable hydrophobicity and transition temperatures of gold nanoparticles coated in 18-crown-6-C-SH moieties by taking advantage of the hole-side cation-diameter relationship. **A.P. Hill**

COLL 179. Temporally decoupled growth and loading of a protein cargo into polymersomes using cellulose paper. **A. Li**, A.B. Subramaniam

COLL 180. *In-situ* spectroscopic ellipsometry as a tool to characterize Cu-ligated mercaptoalkanoic acid multilayers. **A. Patron**, T.J. Mullen, C. Causey

COLL 181. Nanoparticle-templated synthesis of porous carbon for the removal

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of organic pollutants from water. **A.C. Escobosa**, L. Barrera, J. Noveron

COLL 182. Comparison of charge storage properties of prussian blue analogues containing copper and cobalt. **A. Rensmo**, J.R. Hampton

COLL 183. Synthesis of periodic mesoporous organosilicas and related hollow nanostructures. **A.S. Manchanda**, M. Kruk

COLL 184. Chiral recognition of single amino acid surfactants leucine, isoleucine, and norleucine in the presence of diamine counterion with different chain lengths. **A. Benson**, F.H. Billiot, E. Billiot, K.F. Morris

COLL 185. Adsorption on rutile TiO_2 surfaces: Orbital, zero-point energy, and finite-size effects in theoretical models. **A.N. Carlson**, E.S. Gawalt, J.D. Evanseck

COLL 186. Partitioning of limonene into short-chain lecithin dispersions. **A. Karman**, S.R. Dungan, N. Nitin, S.E. Ebeler

COLL 187. Functionalization of CdSe nanoparticles for use in solar nanocomposites. **A. McReynolds**, J.D. Kehlbeck, M.E. Hagerman

COLL 188. Synthetic control over structural and optical properties of Cu(Zn) InS_2/ZnS quantum dots studied at the single particle level. **A. Nguyen**, C.D. Heyes

COLL 189. Coverage ratio of amyloidogenic peptides over nano-gold colloidal particles. **A. Islam**, M. Pujols, E. Okungbowa, P. Shevlin, K. Brown, K. Yokoyama

COLL 190. Brightness optimization of NIR-to-NIR upconversion nanocrystals. **A.M. Chov**, S. May, A. Baride

COLL 191. Exploring interaction between thiolated liposomes and gold/gold coated magnetic nanoparticles. **B. Acharya**, V. Chikan

COLL 192. Spatial distribution of mixtures of electrolytes at the air-water interface for varying temperatures. **B.L. Eggimann**, J.I. Siepmann

COLL 193. Introducing a molecular model system for 5-7 defects in graphene. **B.P. Klein**, N.J. van der Heijden, M. Franke, C.K. Krug, S.R. Kachel, P. Rosenow, F. Posseik, M. Schmid, R. Tonner, I. Swart, C. Kumpf, J. Gottfried

COLL 194. Synthesis, aggregation behavior and enhanced oil recovery performance of an oligomeric nonionic surfactant. **B. Qin**

COLL 195. Extraction of lemon essential oils from lemon peels with food-grade surfactants and its antibacterial applications. L. Huang, **B. Chen**

COLL 196. Density functional theory study of cation adsorption at the capping sites of Keggin-type Al nanoclusters. **B. Hudson**, J.L. Bjorklund, J.W. Bennett, S.E. Mason

COLL 197. G-DNA cancer therapy: Intracellular trafficking in HeLa cells. **B.J. Foster**, K. Fichter

COLL 198. Plasmonic properties and applications of tunable aluminum nanocrescents. **C. Coplan**, M.M. Swartz, J.S. Shumaker-Parry

COLL 199. Systematic study on the gelation properties of simple alkanoic acid metal salts as low molecular mass gelators. **C. Dill**, S. Mathew, A.V. Mallia

COLL 200. Bioconjugation of $CuInS_2$/ZnS quantum dots to FGF and bioimaging their interactions with FGFR. **C. Robinson**, M. Mohale, D. Baucom, A. Nguyen, R.K. Gundampati, M.H. Al-Ameer, S.K. Thallapuranam, C.D. Heyes

COLL 201. Measuring energy transfer efficiency between Au and CdSe nanoparticles. **D. Lara**

COLL 202. Sum frequency generation spectroscopy of partially fluorinated methyl-terminated self-assembled monolayers on gold and UPD-silver surfaces. **D. Rodriguez**, M.D. Marquez, O. Zenasni, S. Baldelli, T. Lee

COLL 203. Study of perfluorophosphonic acid surface modifications on zinc oxide nanoparticles. **D.N. Shoup**, R. Quinones

COLL 204. Degradable cellulose wet adhesives using reductant-responsive microgels. **D. Yang**, R.H. Pelton

COLL 205. Membrane expression of 5-HT_{1B} receptors in N2a cells in response to SSRIs. **E.B. Nowak**, G.K. Illy, K. Fichter

COLL 206. Effect of hydroxide ion concentrations on the binding of montmorillonite to RNA surrogates. **E.P. Gordon**, L. Tribe

COLL 207. Application of electrochromic thin films for electrophysiology. **F. Alfonso**, A.F. McGuire, T. Li, F. Santoro, B. Cui

COLL 208. Single-molecule imaging of serotonin receptor trafficking using quantum dots. **G. Illy**, K. Fichter

COLL 209. New class of nanocatalysts created by coupling of carbon nanotubes, functionalized silica and truncated silver nanoparticle. B.P. Chauhan, **G. Longia**, Q. Johnson, N. Eldabagh

COLL 210. Mild, reproducible and efficient strategy to halogenated sol-gel materials. **G. Longia**, N. Eldabagh, Q.R. Johnson, J. Domena, Y. Xing, **B.P. Chauhan**

COLL 211. Poly(vinyl alcohol) thin film dewetting on polydimethylsiloxane surfaces by directional drying. **H. Nguyen**, Y. Qi, K. Lim, W. Chen

COLL 212. Structure and thermodynamics of worm-like micelles with addition of salt and co-solvent. **H. Jiang**, K. Vogtt, G. Beaucage, M.R. Weaver

COLL 213. Molecular oligonucleotide brushes via ring-opening metathesis polymerization. **H. Lu**, X. Tan, Y. Sun, X. Chen, D. Wang, K. Zhang

COLL 214. Gene expression in a synthetic eukaryotic cell-mimic. **H. Niederholtmeyer**, N.K. Devaraj

COLL 215. Superhydrophobic and hygroscopic surface as an effective anti-icing coating. **H. Nakamura**, T. Yamazaki, M. Tenjimbayashi, S. Shiratori

COLL 216. Silicon-containing dendritic dyes with aggregation-induced emission as fluorescent probes. **H. Wang**, S. Feng, W. Yu

COLL 217. Surface chemistry of carbon nanoparticles functionally select their uptake in various stages of cancer cells. **I. Srivastava**, S.K. Misra, F. Ostadhossein, E. Daza, J. Singh, D. Pan

COLL 218. N-methylmorpholine-N-oxide acts as a 'sacrificial catalyst' to permit imaging of carbon nanodots at the single-particle level. **I. Srivastava**, S.K. Misra, J. Khamo, V. Krishnamurthy, D. Sar, A.S. Schwartz-Duval, K. Zhang, D. Pan

COLL 219. Increasing Zr(IV) ligand binding sites in hetero-metal substituted Well-Dawson polyoxometalates for CWA simulant decomposition. S.L. Giles, J. Lundin, P. Pehrsson, R. Balow, **J.H. Wynne**

COLL 220. Delafossite $CuBO_2$ nanoparticles as an efficient electrocatalyst for water splitting. **J. Pena**, S. Mohan, Y. Mao

COLL 221. Dynamic behavior of thermotropic liquid crystals in coaxial electrospun polyurethane nanofibers. **J. Lundin**, D. Ratchford, Z. Mobley, G.C. Daniels, N. Weise, R. Ananth, R. Casalini, J.H. Wynne

COLL 222. Nanoparticle supercluster formation within crosslinked nanoparticle films: The impact of embedded, coordinating functional groups in crosslinking ligands. **J.A. Dahl**, A.J. Dickenson, M.R. Hammick, A.L. Aakhus

COLL 223. Interparticle spacing in 2-d arrays of covalently-crosslinked, thiol-capped gold nanoparticle films: A function of native ligand shell rigidity, length of crosslinking ligands, and deposition orientation. **J.A. Dahl**, M.M. Metko, Z.S. Walbrun

COLL 224. Characterizing interactions between novel amphiphilic cellulose derivatives and bile salts using quartz crystal microbalance with dissipation monitoring (QCM-D) and surface plasmon resonance (SPR). **J. Zornjak**, D. Novo, K.J. Edgar, C. Fernandez Fraguas

COLL 225. Preparation of crystal-phase-heterostructured 4H/fcc Au@Pd core-shell nanorods for electrocatalytic ethanol oxidation. **J. Liu**, H. Zhang

COLL 226. Surface functionalization of silicone films using click chemistry: Synthetic strategies for designing mechanically tunable surfaces. **J.M. Bradley**, J.M. Taylor, S.A. Morin

COLL 227. Programing the microdynamics of an active particle: From linear to helical trajectories. **J. Lee**, B. Bharti

COLL 228. Investigating the effects of controlled lateral confinement width and surface chemistry on surfactant adsorption onto silica using AFM. **J. Hamon**, B.P. Grady, A. Striolo, R. Tabor

COLL 229. Transfection of unmodified microRNA via ammonium-terminated gold nanoparticles as a platform. **J. Hoang**, S. Patil, T. Liu, A. Palat, P. Gunaratne, T. Lee

COLL 230. Surface plasmons to Zika virus detection: Detection of NS1 protein utilizing localized surface plasmon resonance and surface plasmon resonance spectroscopy. **J.J. Santos**, R.L. Silveira, S.H. Toma, K. Araki, A.G. Brolo, P. Corio

COLL 231. Effects of analyte-induced DNA aptamer conformational changes in aptasensors response. **J.L. Chavez**, P.A. Mirau, J.N. Yoho, J.E. Smith, A. Wissel, J.A. Hagen, N. Kelley-Loughnane

COLL 232. Indolicidin as a model antimicrobial peptide: Investigating their interactions with lipid vesicles and supported bilayers. **J.E. Nielsen**, V. Bjørnestad, T. Lind, H. Jenssen, M. Cardenas, R. Lund

COLL 233. Formation of tethered lipid nanotubes on cellulose paper. **J. Pazzi**, A.B. Subramaniam

COLL 234. Facilitating targeted drug screening: A nanosensor quantifies metabolite-enzyme interactions at the single molecule level. **J. Cheung**, R. Frederiksen, D. Heller

COLL 235. Design and synthesis of multifunctional tungsten sulfide quantum dots for cellular imaging of targeted triple negative breast cancer cells. **K. Gates**, A. Pramanik, P.C. Ray

COLL 236. Hybrid lipid-coated gold nanoparticles for studying axonal transport mechanisms in the retina. **K. Kinnison**, L.J. Wilsey, B.B. Fortune, M.R. Mackiewicz

COLL 237. Self-assembly, gelation studies and mechanotropic properties of molecular gels based on N-phenyloctadecanamides as gelators. **K. Galinat**, E. Begovic, A.V. Mallia

COLL 238. Machine learning dataset and model applied to calculating the Flory-Huggins β parameter. **K.R. Hendrickson**, C. Callaway, S. Venkatram, P. Sood, S. Jang

COLL 239. STEP: Revolutionizing FRET measurement. **K. Akers**

COLL 240. Unidirectional wetting phenomenon on the snake scales. **K. Kawamura**, M. Tenjimbayashi, D. Watanabe, D. Citterio, S. Shiratori

COLL 241. Preparation of monodisperse, supported nanoparticles with switchable surfactants. **K. Bryant**

COLL 242. Investigating organonitrogen pesticides on mineral surfaces via sum frequency generation vibrational spectroscopy. **L. Bromley III**, J. Cartagena, P. Videla, A. Fernando, V.S. Batista, L.A. Velarde

COLL 243. Reliable synthesis of block copolymer templated bimetallic nanoparticles. **L. Knight**

COLL 244. Studies of single-site catalysts on powdered oxide support through self-assembly. **L. Chen**, J. McCann, S.L. Tait

COLL 245. Synthesis and Surface Activity of Gemini Surfactant N,Nβ-bis(octadecyl)-1,4-benzene dimethylpropionate acid. **L. Zhao**, H. Gong, J. Wang

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COLL 246. Fluorescence detection of aggregation of chromonic dyes in the isotropic phase. **L. Zhu**, K.K. Karukstis

COLL 247. Anti-biofouling studies of unsymmetrical oligo(ethylene glycol) spiroalkanedithiol self-assembled monolayer surfaces. **L. St**, J. Craft, P. Chinwangso, H. Lee, M.D. Marquez, T. Lee

COLL 248. Comparing full-wave optical modeling of plasmonic coupling within Au nanoparticle nanoring arrays to structures fabricated via particle lithography. **M. Negrito**, M. Sheldon, J. Batteas

COLL 249. Toward greener synthesis of microcrystalline ZSM-5 Zeolite catalyst and its application in biomass conversion. **M.H. Nada**, S.C. Larsen, E.G. Gillan

COLL 250. Salt mediated synthesis and catalytic activity of para-mercaptobenzoic acid capped monolayer protected gold clusters. R.E. Dufour, **M.G. Rodriguez**, C.L. Heinecke

COLL 251. Designing immobilized radicals to improve dynamic nuclear polarization-enhanced MRI at 6.5 mT. **M.D. Lingwood**, K.E. Maurey, G.A. Shaw, A.K. Sherman, M.S. Rosen

COLL 252. Aggregation of poly-(3-hexylthiophene) at solvent-solvent interfaces. **M. Sapolsky**, D.S. Boucher

COLL 253. Temperature-controlled nano-mite growth on fabricated plasmonic nanostructures. **M.A. Ticknor**, C.A. Lancaster, J.S. Shumaker-Parry

COLL 254. Loading of functional enzymes into giant liposomes using cellulose paper. A.B. Subramaniam, **M. Xu**

COLL 255. Developing the sapphire (0001) surface as a transparent substitute for mica for DNA nanostructure imaging. **M.L. Norton**, M. Rahman, D.P. Neff, Z.T. Boggs

COLL 256. Design of new FMOC and pyrazole-derived nanoparticles for targeting tumorigenic cells. I.A. Banerjee, **M. Hugo**

COLL 257. Synthesis and characterization of Gd:InP/ZnS quantum dots for magnetic resonance imaging. **M. Duszynski**, M. Ellis, K. Fichter

COLL 258. Synthesis and characterization of poly(methacrylic acid) hydrogel fabricated with Ni nanoparticles and investigation of their adsorption and catalytic properties. **M. Ajmal**

COLL 259. Evaluation of spin-casting as a coating method to study dopamine adhesion. **M. Le**, W. Chen

COLL 260. Colloid Chemical Approach to Cracking Formation in Fuel Cell Catalyst Layers. **N. Kumano**, K. Kudo, Y. Akimoto, M. Ishii, H. Nakamura

COLL 261. Nanocomposites of plastic, Silicon polymer and noble metal nanoparticles. **N. Ampomah**, K. Moran, Q. Johnson, **B.P. Chauhan**

COLL 262. Electroless deposition of Nickel on organosilane nanostructures prepared with particle lithography: Characterization with atomic force microscopy combined with magnetic sample modulation. **N. Kuruppu Arachchige**, P.C. Chambers, A.M. Taylor, J.C. Garno

COLL 263. Effect of diamine counterion chain length and pH on the physical properties and chiral recognition ability of amino acid based macromolecular assemblies. **N. Nguyen**, F.H. Billiot, E. Billiot, K.F. Morris

COLL 264. Titania containing thin films for the detection of TATP and peroxide vapors. **N.F. Materer**, A.W. Apblett

COLL 265. P(NiPAM) microgels embedded in p(AAm) hydrogels as sensor. S. Demirci, D. Rees, **N. Sahiner**

COLL 266. Surface ion induced water adsorption on Muscovite mica. **N.N. Lata**, J. Zhou, B. Glatz, S. Sarupria, W.H. Cantrell

COLL 267. Effect of silica interlayer on the plasmonic enhancement of photocatalytic activity. **P. Srinoi**, T. Lee, T. Lee

COLL 268. Synthesis and characterization of gold nanostar particles. **P. Ansari**, T. Lee, R.C. Willson

COLL 269. CdS quantum dot growth dependence on oleylamine concentration. **P.L. Garrett**, N. Razgoniaeva, D. Khon, M. Zamkov

COLL 270. Colloidal synthesis of Fe, Mn and Fe-Mn alloy nanoparticles by rapid inductive heating technique. **P. Sharma**, N. Holliger, V. Chikan

COLL 271. Correlation between hybridization and electrochemical signal in stem-loop E-DNA sensors using single-molecule AFM. **Q. Gu**

COLL 272. Exploring the optical properties of gold nanomites on gold nanotriangles. **R.C. Cocke**, W. Scholl, J.S. Shumaker-Parry

COLL 273. Titanium dioxide-coated plasmonic gold-silver nanoshells. **R. Medhi**, T. Lee, T. Lee

COLL 274. Spectroscopic studies of starvation in *Vibrio cholerae*. **R.D. George**, P. Mosier-Boss, K. Sorensen, A. O'braztsova

COLL 275. Molecular interaction between b-PEI-functionalized gold nanoparticles and *Bacillus subtilis* strains varying in wall teichoic acid composition. **R. Tapia Hernandez**, K.P. Johnson, E.R. Caudill, C.L. Haynes, J.A. Pedersen, V. Feng

COLL 276. Effect of water adsorption on clay mineral interfaces for enhanced gas recovery and CO_2 sequestration: First principles calculations. **R.A. Bennick**, L. Tribe

COLL 277. Design of Development Agent (DA) in latent fingerprint identification. P. Villarreal, I. Villavicencio, **S. Liu**, J. Liu

COLL 278. Selective detection of Pb(II) ion by using a nano material attached aryl-azo-histadine dye. **S. Alamgir**, A. Pramanik, P.C. Ray

COLL 279. Self-assembly of microscale objects using large, double-stranded DNA molecules. **S. Krerowicz**, D.C. Schwartz

COLL 280. Surface adsorption of Nordic aquatic fulvic acid on amine functionalized and non-functionalized mesoporous silica nanoparticles. **S. Jayalath**, V.H. Grassian, S.C. Larsen

COLL 281. Interfacial water structure next to zwitterionic lipids: A vibrational sum frequency spectroscopic study. **S. Pullanchery**, T. Yang, P.S. Cremer

COLL 282. Titania stabilized cuprous oxide photocatalyst for the reduction of carbon dioxide. **S. Alden**, D.A. Rider

COLL 283. Investigation of chiral recognition of dipeptide based micellar systems. **S. Tubbs**, E. Billiot, K.F. Morris, F.H. Billiot

COLL 284. Comparing electrochemical calculations and particle induced x-ray emission measurements of Prussian blue analogue deposits. **S.D. Joffre**, J.R. Hampton

COLL 285. Synthesis and physicochemical properties of a novel carboxylbetaine-type surfactants containing benzene ring. **S. Gao**, Q. Jiang, Z. Song, F. Lan

COLL 286. Structural investigation on the mechanism of the endosomal escape by pH-sensitive Gemini surfactants. **S. Chang**, Y. Chen

COLL 287. Probing the interactions between small molecules and phospholipids at the biointerface. **S. Sun**, A. Sendecki, S. Pullanchery, D. Huang, T. Yang, P.S. Cremer

COLL 288. Self-assembled monolayers derived from symmetric olefin-bridged bidentate adsorbates on gold. **S. Sakunkaewkasem**, T. Lee, M.D. Marquez, O. Zenasni

COLL 289. Study of the excited state processes of 1,3,6,8-Tetrakis(trimethylsilylethynyl)pyrene in monomer and aggregated state. **S. S**, S. Sankararaman, P. Edamana

COLL 290. Probing the interaction of enzyme and gold nanoparticles with various coatings. **S. Neupane**, Y. Pan, Z. Yang

COLL 291. Programmable preparation of three-dimensional assembly of gold triangular nanoprisms for biosensing applications. **T. Habarakada Liyanage**, S. Shaffer, H. Nguyen, R. Sardar

COLL 292. Elucidating the time-dependent photoluminescence properties of colloidal carbon dots. **T. Chu**, D. Gerrity, S. Chatterjee

COLL 293. Surface functionalization with glycopolymers for selective adherence of the bacteria *Shewanella oneidensis*. **T.D. Young**, W. Liau, C. Lee, G. Wong, A. Kasko, P.S. Weiss

COLL 294. Liquid-phase epitaxial growth of triangular Au nanoplates on MoS_2 nanosheet for electrocatalytic hydrogen evolution. **T. Tran**, **H. Zhang**

COLL 295. Self-assembled monolayers derived from the adsorption of phenyl- and perfluorophenyl-terminated alkanethiols on gold. **T. Yu**, T. Lee, M.D. Marquez, O. Zenasni

COLL 296. Towards continuous *in situ* sensing of marine pollutants using surface enhanced Raman spectroscopy (SERS). **T. Küster**, G.D. Bothun

COLL 297. Sulfur@Gold@Titanium dioxide yolk-shell nanoparticles for lithium-sulfur battery applications. **T. Liu**, T. Lee

COLL 298. Promotion effect of alklyamine functionalized silica on embedded gold nanoparticle hydroaminations. **T. Graham**, A. Rosul, D. Wu, S.R. Saunders

COLL 299. Single particle fluorescence studies of semiconductor nanoparticles alloyed by kinetic control. **T. Hull**, J.S. Owen

COLL 300. Magnetron sputtering of gold thin films under ambient conditions and manipulation of deposition. **T.J. Adams**, B. Evans, C. Miller, I. Seneviratne

COLL 301. Synthesis and characterization of organosoluble $Au_{36}(SPhCH_3)_{24}$ nanomolecules. **V. Ganeshraj**

COLL 302. Nanomite-decorated nanoparticles as surface-enhanced spectroscopy substrates. **W.E. Scholl**, C.A. Lancaster, M.A. Ticknor, J.S. Shumaker-Parry

COLL 303. Multicolor carbon dots based on solvatochromism. H. Wang, P. Haydel, L. Earb, S. Wang, **W. Yu**

COLL 304. Construction of hybrid alginate nanogels loaded with manganese oxide nanoparticles for enhanced tumor MR imaging. W. Sun, J. Zhang, C. Zhang, P. Wang, C. Peng, M. Shen, **X. Shi**

COLL 305. Withdrawn

COLL 306. Organize gold nanoparticles by DNA origami cage. **Y. Zhang**

COLL 307. Charge-reversal amphiphiles induced by pH: Distinctive interaction with normal and cancer cells. **Y. Chang**, Z. Huang, J. Xu, X. Zhang

COLL 308. Effect of oil droplet size on stability of concentrated oil-in-water emulsion with unsaturated fat. M. Shinada, **Y. Watanabe**

COLL 309. Preparation of angle-independent color materials by applying Mie resonances. **Y. Naoi**, Y. Takeoka, T. Seki

COLL 310. Self-assembled polydopamine coatings via drop casting. **Y. Zhou**, W. Chen

COLL 311. Novel synthesis of bispectral obscurant smoke. **Z. Zander**, D. Kuhn, A. Polk

COLL 312. Pentamer substrate for reproducible surface enhanced raman spectroscopy. **Z. Petrek**, U. Paez, T. Ye

COLL 313. Withdrawn

COLL 314. Developing a technique to determine the packing density of a lipid bilayer and exploring the effect of packing density on membrane fusion. **Z. Liu**, Y. Chen

COLL 315. Influences of surface chemistry and nanoscopic roughness on the frictional

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properties of MoS_2 nanosheets. **Z. Liu**, J. Batteas

COLL 316. Applications of nanotechnology in bone tissue regeneration. **J. Santillan**

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 242

ACS Award in Colloid Chemistry: Symposium in honor of Håkan Wennerström

U. Olsson, N.J. Wagner, *Organizers, Presiding*

8:30 COLL 317. Controlling water evaporation through self-assembly. **E. Sparr**, K. Roger, D. Topgaard, H. Wennerström, D. Pham, S. Björklund

9:00 COLL 318. Self-assembly of block copolymers in ionic liquids: Mixed pluronics- structure, rheology and use as wearable electronics. **N.J. Wagner**, R. Chen, C. Lopez-Barron

9:30 COLL 319. Lowering of surface tension of water by surfactants: principles of molecular design. **A. Kabalnov**

10:00 Intermission.

10:10 COLL 320. Kinetic stability of non-ionic surfactant vesicles. A.P. Schroder, J. Crassous, C.M. Marques, **U. Olsson**

10:40 COLL 321. Lipid materials processing: The emergence of super-swelled membrane single-crystals. **C. Leal**

11:10 COLL 322. Physicochemical code for protein interactions in live cells. **M. Oliveberg**

11:40 COLL 323. Protein aggregation and gelation – insight from combining scattering, rheology and computer simulations. **A. Stradner**

Section B
Ernest N. Morial Convention Center
Room 245

2018 Priestley Medalist: Symposium in honor of Geraldine Richmond

R.A. Walker, *Organizer*
S. Wren, *Presiding*

8:30 Introductory Remarks.

8:35 COLL 324. Flipping out (or in) over lipids. **J.C. Conboy**

9:05 COLL 325. In your face: Adventures in computational vibrational sum-frequency spectroscopy. **N.A. Valley**

9:35 Intermission.

9:55 COLL 326. Oh, the places you'll go: Chemical structure, organizations and reactivity in asymmetric environments. **R.A. Walker**

10:25 COLL 327. Science, serendipity and sustainability. **B. Chase**, I. Noda, J.F. Rabolt

10:55 COLL 328. Making the rounds: Molecular characterization of surfactant stabilized nanoemulsion surfaces. **G.L. Richmond**

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A.N. Parikh, *Organizers*
D.L. Daleke, D.Y. Sasaki, *Presiding*

8:30 COLL 329. Photo-induced pinocytosis for artificial cell feeding. **D. Konetski**, D. Zhang, C. Bowman

8:50 COLL 330. *In situ* determination of membrane protein orientation. **Z. Chen**

9:20 COLL 331. Cellulose paper assembles vesicles from fatty acids and amphiphilic block copolymers. **A.B. Subramaniam**, A. Li, J. Pazzi, M. Xu

9:50 COLL 332. Bacteriorhodopsin membrane entrapped within photocatalytic amorphous titania. K.E. Johnson, S. Gakhar, S.H. Risbud, **M.L. Longo**

10:20 COLL 333. Designing size-controllable bicelles. C. Mandelkern, Y. Liu, I. Alahmadi, K. Chih, J. Fang, **M. Nieh**

10:50 COLL 334. Assessing the structure and stability of transmembrane oligomeric intermediates of an alpha-helical toxin. R. Desikan, P.K. Maiti, **G.K. Ayappa**

11:20 COLL 335. *Bacillus subtilis* lipid extract, a branched-chain fatty acid model membrane. **J. Nickels**, S. Chatterjee, B. Mostofian, C.B. Stanley, M. Ohl, P. Zolnierczuk, R. Schulz, D.A. Myles, R.F. Standaert, X. Cheng, J. Katsaras

11:50 COLL 336. Monitoring and modulating ion traffic in hybrid lipid/polymer vesicles. **W. Paxton**, P. McAninch, K. Achyuthan, S. Shin, H. Monteith

Section D
Ernest N. Morial Convention Center
R06

Chemistry of Molecular Electronics

Molecular-Scale Electronics

Cosponsored by PHYS
M.S. Inkpen, G.C. Solomon, L. Venkataraman, *Organizers, Presiding*

8:30 COLL 337. New molecules for single-molecule electronics in break junction devices. **M.R. Bryce**

9:00 COLL 338. Photovoltaic response observed in thin molecular bilayer rectifiers with symmetric carbon contacts. **S.R. Smith**, R.L. McCreery

9:20 COLL 339. Molecular silicon electronics. **R.S. Klausen**

9:50 COLL 340. Insulated molecular wires: Inhibiting orthogonal contacts in metal complex. **D. Costa Milan**, O.A. Al-Owaedi, S. Bock, M.C. Oerthel, M.S. Inkpen, D.S. Yufit, A.N. Sobolev, N.J. Long, T. Albrecht, S.J. Higgins, M.R. Bryce, R. Nichols, C.J. Lambert, P.J. Low

10:10 COLL 341. Quantum interference based single-molecule insulators. **L. Venkataraman**

10:30 Intermission.

10:40 COLL 342. Single-molecule electronic components based on molecular design. **H. van der Zant**

11:10 COLL 343. Resonant tunneling transport in single-molecule junctions. **Y. Zang**, S. Ray, A. Borges, E. Fung, G.C. Solomon, S.A. Patil, L. Venkataraman

11:30 COLL 344. Solution processable nanocarbon hybrids for single-molecule investigations. **M. Palma**

11:50 COLL 345. Two-terminal single-molecule functional devices. **E. Scheer**, S.G. Bahoosh, J.C. Cuevas, A. Erbe, S. Hambsch, R. Hayakawa, C. Herrmann, T. Huhn, M.A. Karimi, Y. Kim, M. Matt, P. Nielaba, F. Pauly, C. Schirm, T. Sendler, D. Sysoiev, D. Weber, J. Wolf, M.S. Zöllner

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
M. Cai, H. Fan, Y. Han, *Organizers*
F. Bai, *Organizer, Presiding*
H. Fan, *Presiding*

8:30 COLL 346. Colloidal synthesis of nanomaterials: challenges and opportunities. A. Hazarika, V. Srivastava, H. Zhang, **D. Talapin**

9:00 COLL 347. Programmable nanoparticle systems: designed architectures, controlled processes and regulated functions. **O. Gang**

9:30 COLL 348. Self-assemblies of graphene quantum dots: From hollow nanoshells to the origin of life. **Z. Qu**, N. Kotov

9:50 COLL 349. Perspectives in nanoscale chemistry. **A. Vartanian**

10:10 Intermission.

10:30 COLL 350. Synthesis and assembly of plasmonic metal oxide nanocrystals. **D.J. Milliron**

11:00 COLL 351. Synthesis and optical interaction in janus au-silica-quantum dot hybrid nanostructures. Y. Luo, **J. Zhao**

11:30 COLL 352. Geometric influence on photoelectrocatalytic properties of assembled ZnO nanonetwork. **Y. Mao**

11:50 COLL 353. Computational survey of counterions and capping groups in Al nanoclusters. **S.E. Mason**, B. Hudson, J.L. Bjorklund, J.W. Bennett

12:10 COLL 354. Adsorption of small cationic nanoparticles onto large anionic particles from aqueous solution: A model system for understanding pigment dispersion and the problem of effective particle density. **S. North**, E. Jones, G. Smith, O. Mykhaylyk, T. Annable, S.P. Armes

Section F
Ernest N. Morial Convention Center
R09

Fundamental Studies of Mechanochemical & Tribochemical Processes at Interfaces

J.D. Batteas, W.T. Tysoe, *Organizers*
R.M. Espinosa-Marzal, *Organizer, Presiding*

8:30 COLL 355. Force transduction at cell-to-cell adhesive contacts. **D.E. Leckband**, S. Barrick, X. Kong, E. Tajkhorshid

9:00 COLL 356. Tribology of biomimetic patterned polymer textures as skin coating models. R. Jin, X. Xu, C. Cazeneuve, J.C. Chang, **M. Ruths**, G.S. Luengo

9:20 COLL 357. Anomalous potential dependent friction on Au (111) measured by AFM. **L. Pashazanusi**, N. Pesika

9:40 COLL 358. Nanofriction and surface nanomechanical properties of cotton (*Gossypium hirsutum* L.) fibers as studied with contact mode and force-distance curve-based AFM. **F. Hosseinali**, J.A. Thomasson, J.D. Batteas

10:00 COLL 359. What does mucin do for the cornea? *In vitro* measurements of mucin structure on an epithelial monolayer. **T. Angelini**

10:30 Intermission.

10:45 COLL 360. Promise of stable nanocrystalline metals: Ultra-low wear and diamond-like carbon from thin air. **N. Argibay**, M. Chandross, P. Lu, D. Adams, M. Dugger, T. Babuska, J. Curry, A. Kustas, T. Furnish, B. Boyce, B. Clark

11:15 COLL 361. Structural superlubricity of platinum and gold under ambient conditions: The effects of chemistry and geometry. A. Özoğul, E. Cihan, S. Ipek, E. Durgun, **M.Z. Baykara**

11:35 COLL 362. Size-dependent pseudo-elasticity in gold nanocrystals. **L. Hanson**, X. Gu, C. Eisler, M. Koc, P. Alivisatos

11:55 COLL 363. Wear-induced chemical nanolayering and its beneficial impact on wear resistance. **P. Bellon**

Section G
Ernest N. Morial Convention Center
Room 203

Nanomaterials

Novel Synthesis & Nanostructures

J.A. Hollingsworth, R. Nagarajan, *Organizers*
J. Macdonald, *Presiding*

8:30 COLL 364. Indium phosphide quantum shells tunable through visible and near infrared. **A.M. Dennis**

9:00 COLL 365. Indium phosphide clusters as precursors to novel nanoscale phases. **B.M. Cossairt**, M. Friedfeld, J. Stein, A. Ritchhart

9:30 COLL 366. Nanosheets and emulsion systems. **H.V. Kumar**, C.D. Liyanage, T. Francis, D.H. Adamson

9:50 COLL 367. Purification and *in situ* ligand exchange of metal-carboxylate-

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treated fluorescent InP quantum dots via gel permeation chromatography. **A. Roberge**, J. Stein, Y. Shen, B.M. Cossairt, A.B. Greytak

10:10 COLL 368. Development of sequence-dependent structure/function relationships for peptide-enabled nanomaterials. **N. Bedford**

10:30 COLL 369. Nanoparticle chemistry in solution observed by time-resolved 3D TEM. B. Kim, J. Heo, J. Kim, **J. Park**

10:50 COLL 370. Crystal structure of Faradaurate-279: $Au_{279}(SPh\text{-}tBu)_{84}$ nanomolecules. **N. Sakthivel**, S. Theivendran, V. Ganeshraj, A.G. Oliver, A. Antonysamy

11:10 COLL 371. Core size interconversions of gold nanomolecules: $Au_{30}(S\text{-}tBu)_{18}$ and $Au_{36}(SPhX)_{24}$. **T.C. Jones**, A. Antonysamy, S. Theivendran, L. Sementa, A. Fortunelli

11:30 COLL 372. Imidazolium ionic liquids as multifunctional solvents, ligands, and reducing agents for noble metal deposition onto well-defined heterostructures, and the effect of synthetic history on catalytic performance. **M.D. Ballentine**, M. Garcia, LJ. Hill

Section H
Ernest N. Morial Convention Center
Room 204

Surface Chemistry

Molecules on Surfaces

S.L. Tait, *Organizer*
J.R. Hampton, B. Schuler, *Presiding*

8:30 COLL 373. Molecular coupling between organic molecules and metal. **H. Pengcheng**, X. Lu, Z. Chen

8:50 COLL 374. Ullmann coupling of helical polycyclic aromatic hydrocarbons on metal surfaces. **A. Mairena**, M. Parschau, J. Seibel, M. Wienke, L. Zoppi, C. Wäckerlin, J. Li, K. Martin, N. Avarvari, A. Terfort, K. Ernst

9:10 COLL 375. Redox-active ligand controlled selectivity of vanadium oxidation on Au(100). **S.L. Tait**, C. Tempas, T.W. Morris, D. Wisman, N. Din, D. Le, C.G. Williams, M. Wang, A.V. Polezhaev, T.S. Rahman, K.G. Caulton

9:40 COLL 376. Electrical and optical studies of porphyrin-based two-dimensional metal-organic frameworks. **K. Ishihara**, F. Tian

10:00 COLL 377. Molecular topology and surface chemical bond: Alternant vs. non-alternant aromatic molecules. **B.P. Klein**, N.J. van der Heijden, M. Franke, C.K. Krug, S.R. Kachel, P. Rosenow, F. Posseik, M. Schmid, R. Tonner, I. Swart, C. Kumpf, J. Gottfried

10:20 Intermission.

10:40 COLL 378. Characterization of electrogenerated hexacynoferrate thin films for battery applications. S.D. Joffre, A. Rensmo, **J.R. Hampton**

11:10 COLL 379. Measuring individual point defects in monolayer WS_2 using scanning probe microscopy. **B. Schuler**, C. Kastl, C. Chen, S. Refaely-Abramson, S. Yuan, R. Roldan, N.J. Borys, T. Kuykendall, F. Ogletree, J. Neaton, S. Aloni, A. Schwartzberg, A. Weber-Bargioni

11:30 COLL 380. Structure and defects in the TiN-TiO2 rutile interface. J. Gutierrez, **M. Nolan**

12:00 COLL 381. Fundamental surface modification and synchrotron-based spectroscopy of nanoscale diamond with amines, boranes and silica. G. Jean-Pierre, P. Tran, P.J. Sandoval, J. Hnatek, A. Arreola, A. Len, C. Melendrez, D. Barrera, R. Robinson, P. Yamaguchi, K. Lopez, A. Hernandez, E. Favre, D. Nordlund, V. Altoe, **A. Wolcott**

Section I
Ernest N. Morial Convention Center
Room 205

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Surface Modification & Function

Cosponsored by WCC
A.V. Teplyakov, *Organizer*
H. Lee, *Organizer, Presiding*

8:30 COLL 382. Electrochemical sensor of CO_2 based on surface modified halloysite nanotubes. **C. Prasittichai**

9:00 COLL 383. Functionalizing silicon surfaces: mechanistic connections between molecules and interfaces. **J.M. Buriak**, M. Hu, T. Hauger

9:30 COLL 384. Probing organic reactions at surfaces using DART-MS. **H. Zuilhof**

10:00 Intermission.

10:15 COLL 385. Fe-based modification of graphite felt surfaces for electrochemical treatment of aqueous contaminants. **M. Kong**

10:45 COLL 386. Metal contacts in silicon solar cells: Role of surface science. **K. Roelofs**

11:15 COLL 387. Nanoparticles via vapor phase condensation for energy applications. **B.M. Clemens**, B. Gibbons, M. Wette, D. Higgins, T.F. Jaramillo, J. Baker, S.F. Bent, A. Mehta, R. Davis

Elucidation of Mechanisms & Kinetics on Surfaces

Theory

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Assembly & Colloidal Interactions of Cellulose Nanocrystals
Sponsored by CELL, Cosponsored by COLL

Physical Chemistry of Ionic Liquids

Electrochemistry and Electrochemical Interfaces
Sponsored by PHYS, Cosponsored by COLL‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 242

ACS Award in Colloid Chemistry: Symposium in honor of Håkan Wennerström

U. Olsson, N.J. Wagner, *Organizers*
C. Leal, A. Stradner, *Presiding*

2:00 COLL 388. Thermorsponsive colloidal molecules with tunable directional interactions. **P. Schurtenberger**

2:30 COLL 389. Colloidal and macromolecular complexes at fluid-fluid interfaces and impact on mechanical properties. M.L. Davidson, S.M. Kirby, **L. Walker**

3:00 COLL 390. Stratification in colloidal films: Experimental evidence from atomic force microscopy and small-angle x-ray scattering. A. Carr, W. Liu, X. Liu, K. Yager, A.F. Routh, **S. Bhatia**

3:30 Intermission.

4:00 COLL 391. Structure and dynamics of nanoparticles in polymeric fluids. R. Poling-Skutvik, R. Krishnamoorti, **J. Conrad**

4:30 COLL 392. Cascade processes in "artificial cells" triggered by light, chemicals, or enzymes. **S.R. Raghavan**, K.C. DeMella

5:00 COLL 393. Herpesvirus infectivity facilitated by internal DNA pressure and capsid stability. **A. Evilevitch**

Section B
Ernest N. Morial Convention Center
Room 245

2018 Priestley Medalist: Symposium in honor of Geraldine Richmond

R.A. Walker, *Organizer*
N.A. Valley, *Presiding*

2:00 COLL 394. Impact of atmospheric aerosols and clouds on hydrocarbon chemistry. **J.S. Francisco**

2:30 COLL 395. From the field to the lab: Atmospheric organics in urban air and at the air-water interface. **S. Wren**, G.L. Richmond, J. Brook, B. Gordon, K. Hayden, J. Liggio, G. Lu, C. Mihele, R. Mittermeir, N.A. Valley, J. Wentzell

3:00 COLL 396. Towards predictive separations using 4D super-resolution microscopy. **C.F. Landes**

3:30 Intermission.

3:50 COLL 397. Solvent isotope effect on biomolecular adsorption at hydrophobic surfaces. T. Jarisz, K. Jena, M. Dixon, **D.K. Hore**

4:20 COLL 398. Maximizing efficiency – practical approaches to linking titration (and other methods) with NIR spectroscopy. **A. Hopkins**

4:50 COLL 399. Unraveling chemical processes from a metrology perspective. **P. Chu**

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, *Organizers*
A.N. Parikh, *Organizer, Presiding*
K. Morigaki, *Presiding*

2:00 COLL 400. Interactions between charged nanoparticles and giant vesicles fabricated from inverted-headgroup lipids. **L. Wang**, N. Malmstadt

2:20 COLL 401. Adenosine receptor 2A phase segregation behavior depends on its ligand binding state. **N. Malmstadt**

2:50 COLL 402. Measurement of flippase activity in individual red blood cells. M. Hosek, **D.L. Daleke**

3:20 COLL 403. Interaction of G protein transducin with GPCR rhodopsin studied by SANS. O. Soubias, J. Nickels, A. Yeliseev, K.G. Hines, W.E. Teague, J.K. Northup, J. Katsaras, **K. Gawrisch**

3:50 COLL 404. Imaging membrane-interacting peptides via a fluorescent amino acid. **F. Gai**

4:20 COLL 405. Time-resolved imaging of molecular transport through living cell membrane. **H. Dai**

4:50 COLL 406. Ytterbium ions strongly inhibit lipid flip-flop. V. Cheng, D. Wang, **J.C. Conboy**

Section D
Ernest N. Morial Convention Center
R06

Chemistry of Molecular Electronics

Molecular-Scale Electronics

Cosponsored by PHYS
M.S. Inkpen, G.C. Solomon, L. Venkataraman, *Organizers, Presiding*

2:00 COLL 407. Towards self-assembled single-molecule electronic devices. **K. Moth-Poulsen**

2:30 COLL 408. Tuning the polarity of charge carriers using electron deficient thiophenes. **J. Low**, B. Capozzi, J. Cui, S. Wei, L. Venkataraman, L.M. Campos

2:50 COLL 409. All-carbon molecular electronics for the real world. **R.L. McCreery**, A. Bergren, A.M. Najarian, M. Supur, S.R. Smith, U. Tefashe

3:20 COLL 410. Organometallic self-assembled monolayer films of linear azulenic and biazulenic p-linkers featuring asymmetric anchoring. **M.k. Okeowo**, C.L. Berrie, M.V. Barybin

3:40 COLL 411. Large-area molecular electronic devices employing graphene materials as soft top-contacts. **K.**

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Nørgaard

4:10 Intermission.

4:20 COLL 412. Carbon electrode-molecule junctions: A reliable platform for molecular electronics. **X. Guo**

4:50 COLL 413. Structural design of single-molecule junctions with electromechanical switching properties. **A. Vezzoli**, K. Wang, A. Ismael, I. Grace, C.J. Lambert, B. Xu, S.J. Higgins, R. Nichols

5:10 COLL 414. Toward nanoscale rotoelectronics: A trigonal array of dipolar molecular rotors. T.F. Magnera, J. Kaleta, P.I. Dron, J. Wen, C. Zhu, C.T. Rogers, **J. Michl**

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
M. Cai, H. Fan, Y. Han, *Organizers*
F. Bai, *Organizer, Presiding*
H. Fan, *Presiding*

2:00 COLL 415. Bismuth oxide thin films. **S.E. Rodil**, C.L. Gomez, O. Depablos-Rivera, J.C. Medina

2:30 COLL 416. Self-assembly of quantum dot gold hetero-structural nanocrystals and their transformations under high pressure. **O. Chen**, **H. Zhu**, **Y. Nagaoka**, Z. Wang

3:00 COLL 417. Role of planar defects during the synthesis of stellated plasmonic nanocrystals. **J.D. Smith**, K.M. Koczkur, J.A. Burkhart, S.E. Skrabalak

3:20 Intermission.

3:30 COLL 418. Reconfigurable plasmonic nanoparticle assemblies. **D.S. Ginger**

4:00 COLL 419. *In situ* observation of nucleation and growth of nanocrystals. **H. Weller**

4:30 COLL 420. Postsynthetic surface treatments for essentially trap-free $CsPbBr_3$ colloidal nanocrystals. **B.A. Koscher**, J.K. Swabeck, N. Bronstein, P. Alivisatos

4:50 COLL 421. Modeling of nanoparticle superlattices self-assembly at liquid-air interfaces. **L. Vukovic**

5:10 COLL 422. Facile fabrication of spiky gold-carbon black nanoshells for efficient surface-enhanced Raman scattering. **A. Abbasi**, T. Küster, A. Bose, G.D. Bothun

Section F
Ernest N. Morial Convention Center
R09

Fundamental Studies of Mechanochemical & Tribochemical Processes at Interfaces

J.D. Batteas, R.M. Espinosa-Marzal, W.T. Tysoe, *Organizers*
J.R. Felts, *Presiding*

2:00 COLL 423. Friction regimes of water-lubricated diamond (111): Role of interfacial ether groups and tribo-induced aromatic surface reconstructions. **M. Moseler**

2:30 COLL 424. Examination of bonding using molecular dynamics and *in-situ* nanoindentation. **J.A. Harrison**

3:00 COLL 425. Titania lubrication using oil-ionic liquid mixtures. H. Li, P. Cooper, A. Somers, M.W. Rutland, P. Howlett, **R. Atkin**

3:20 COLL 426. Boundary lubrication studied by resonance shear measurement. **K. Kurihara**, M. Mizukami, M. Kasuya

3:40 COLL 427. Mechanochemistry enables a rational, targeted synthesis of mixed-metal microporous metal-organic frameworks. **G. Ayoub**, K. Uzarevic, A. Howarth, L.S. Germann, R.E. Dinnebier, O. Farha, T. Friscic

4:00 Intermission.

4:15 COLL 428. Atomic-scale insights into contacts between nanoscale bodies: *In situ* experiments and matched atomistic simulations. **T.D. Jacobs**, S. Vishnubhotla, S.R. Khanal, R. Chen, X. Hu, A. Martini

4:45 COLL 429. Tribochemical reactions in nanoscale lubrication and wear. **R. Carpick**

5:15 COLL 430. Mechanochemistry in high shear stress elastohydrodynamic contacts. j. zhang, **H.a. Spikes**

5:45 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 203

Nanomaterials

Nanocrystal Assembly

J.A. Hollingsworth, R. Nagarajan, *Organizers*
J. Vela, *Presiding*

2:00 COLL 431. New chalcogenide aerogel compositions from covalent crosslinking + ion-exchange. I. Hewavitharana, **S. Brock**

2:30 COLL 432. Cascade synthesis of binary nanoparticles polymer composites. K.W. Kwock, H.D. Magurudeniya, A.J. Singh, J.A. Hollingsworth, **M.A. Firestone**

3:00 COLL 433. Pressure-induced nanoparticle assemblies. **H. Fan**

3:30 COLL 434. Emulsification of two-dimensional nanosheets: from exfoliation to functional liquids and composites. **S. Ogilvie**, M. Large, A. King, A. Dalton

3:50 COLL 435. Silver nanowire networks for transparent film heaters: Synthesis, nanoscale characterization and integration in functional devices. **J. Simonato**

4:10 COLL 436. Hydrogel with embedded chemical gradient for analyte collection on surface enhanced infrared absorption spectroscopy. **S. Zhang**, H. Chen, P.V. Braun

4:30 COLL 437. Withdrawn

4:50 COLL 438. Comparing the rheo-optics of aqueous sulfonated cellulose nanocrystal and model cholesteric dispersions. **M.M. Noor**, P. Saha, M. Pospisil, M.J. Green, V.A. Davis

5:10 COLL 439. Surface templating and entropy-driven effect to the self-assembly of protein 2D crystal at solid-liquid interface. **S. Zhang**, R. Alberstein, F.A. Tezcan, J.J. DeYoreo

Section H
Ernest N. Morial Convention Center
Room 204

Surface Chemistry

Reactions at Surfaces

S.L. Tait, *Organizer*
R. Barbosa, J. De Roo, *Presiding*

2:00 COLL 440. Preparing and modifying Fischer-Tropsch catalysts through metal oxalate route. **R. Barbosa**, Y. Xiang, N. Kruse

2:50 COLL 441. Surface Chemistry on Single Hot Carbon Nanoparticles. B.A. Long, D.J. Rodriguez, **S.L. Anderson**

3:20 COLL 442. Metal vapor adsorption calorimetry on calcium niobate nanosheets: Energetics and adsorbate structure. **W. Zhang**, J.E. Eichler, R. Uppuluri, T.E. Mallouk, C.T. Campbell

3:40 Intermission.

4:00 COLL 443. Withdrawn

4:30 COLL 444. *Ab initio* molecular dynamic study about effect of acid-base molecule adsorption on acidity on ZrO_2 surface. **R. Sato**, Y. Shibuta, F. Shimojo, S. Yamaguchi

4:50 COLL 445. Surface chemistry of group 4 metal oxide nanocrystals. **J. De Roo**, K. De Keukeleere, F. Delpech, Y. Coppel, I. Van Driessche, J.C. Martins, J.S. Owen, Z. Hens

Section I
Ernest N. Morial Convention Center
Room 205

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Interfaces & Assembly: From Molecular Understanding to 3D Materials

Cosponsored by WCC
H. Lee, A.V. Teplyakov, *Organizers*
A.L. Harris, *Presiding*

2:00 COLL 446. Hybrid interfaces via organic chemistry on semiconductors. L. Pecher, **R. Tonner**

2:30 COLL 447. Lateral interactions between organic molecules on solids: Recent examples from functionalization of the Ge(100)-2×1 surface. **B. Shong**

3:00 COLL 448. Surface chemical choreography of vapor-liquid-solid semiconductor nanowire synthesis. **M. Filler**

3:30 COLL 449. III-Nitride nanostructures for photonics and beyond. **G.T. Wang**

4:00 Intermission.

4:15 COLL 450. Molecular design and chemical modification of semiconductor surfaces. **A.V. Teplyakov**

4:45 COLL 451. Tailoring aerogels for energy storage and sensing applications. **M.A. Worsley**

5:15 COLL 452. In honor of Prof. Stacey Bent: Self-assembly across substrates. **P.S. Weiss**

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Assembly & Colloidal Interactions of Cellulose Nanocrystals
Sponsored by CELL, Cosponsored by COLL

Physical Chemistry of Ionic Liquids

Electrochemistry and Electrochemical Interfaces

Sponsored by PHYS, Cosponsored by COLL‡

Magnetically Recoverable Catalysts
Sponsored by CATL, Cosponsored by COLL, ENFL and INOR

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
R. Nagarajan, *Organizer*

8:00–10:00

47, 133, 160, 177, 182-185, 191-192, 197, 200, 202, 204, 207-208, 212-214, 217, 222, 224, 227-232, 235, 242, 244-245, 247-249, 251, 255-258, 260, 262-263, 265-266, 270- 271, 273-274, 276, 278-280, 283-284, 287, 289-291-293, 296, 298, 306, 309, 312, 315-316, 357-358, 362, 423, 427-428. See previous listings.

566. See subsequent listings.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center

‡*Cooperative Cosponsorship*

Room 242

ACS Award in Colloid Chemistry: Symposium in honor of Håkan Wennerström

U. Olsson, N.J. Wagner, *Organizers*
S. Bhatia, E. Sparr, *Presiding*

8:30 COLL 453. Hydration repulsion between polar surfaces and lipid membranes: Insights from solvent-explicit molecular dynamics simulations. **E. Schneck**, M. Kanduc, B. Kowalik, A. Schlaich, R. Netz

9:00 COLL 454. Molecular thermodynamic modeling of interactions between alpha-helical peptides and lipid bilayer membranes. **R. Nagarajan**

9:30 COLL 455. Double layer forces and the dielectric approximation. **L. Pegado**, B. Jönsson, H. Wennerström

10:00 COLL 456. Self-regulation and amplification of ion permeation. **H. Moehwald**, J. Duhamet, M. Pleines, T. Zemb

10:30 Intermission.

10:40 COLL 457. Surface forces measurement for materials science. **K. Kurihara**

11:10 COLL 458. From polymeric to oligomeric stabilization of colloidal spheres. **J. Bergenholtz**

11:40 COLL 459. Nanoporous polymer sponges. **R. Strey**

Section B
Ernest N. Morial Convention Center
Room 245

Biomaterials & Biointerfaces

DNA at Materials Interfaces

V. Gordon, *Organizer*
A.P. Goodwin, *Organizer, Presiding*

8:30 COLL 460. Molecular simulation of single nucleotides moving through nanoslits composed of self-assembled monolayers terminated with various chemical groups. X. Tong, **B. Novak**, D. Moldovan

8:50 COLL 461. Charge-reversal nanocarriers for cancer gene delivery. **Y. Shen**

9:10 COLL 462. Self-assembled spherical nucleic acids from oligonucleotide-polymer conjugates for drug delivery and immunotherapy. **K. Zhang**

9:30 COLL 463. Carbonano-tweezers for twisting DNA duplex in cancer cells. **I. Tripathi**, S.K. Misra, F. Ostadhossein, I. Srivastava, D. Pan

9:50 Intermission.

10:10 COLL 464. Combining peptide arrays and mass spectrometry for high throughput experiments. **M. Mrksich**

10:40 COLL 465. Bio-nano interfaces for renewable energy. **J. Cha**

11:10 COLL 466. Reagentless DNA bioconjugation to metal surfaces. **A.L. Furst**, M.B. Francis

11:30 COLL 467. Evidence for DNA as a biomimetic template in calcium phosphate mineralization. **A.E. Gerdon**

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A.N. Parikh, *Organizers*
K. Gawrisch, N. Malmstadt, *Presiding*

8:30 COLL 468. Cargo release mechanics of lipid bilayer coated mesoporous silica nanoparticles. **D.Y. Sasaki**, C. Dolstra, A. Noureddine, J. Brinker

9:00 COLL 469. Nanometric gap structure for selective biosensing created with patterned lipid bilayer, silicone elastomer, and silica nanoparticles. **K. Morigaki**, M. Tanabe, R. Komatsu, K. Ando

9:30 COLL 470. Probing ion and small molecule drug interactions with lipid membranes. **P.S. Cremer**, S. Sun, S. Pullanchery

10:00 COLL 471. Compressible simulation model for lipid bilayer membranes: Faithful treatment of surface tension at the continuum level. **F.L. Brown**

10:30 COLL 472. Recent advances in the *in situ* synthesis of phospholipid membranes. **N.K. Devaraj**

11:00 COLL 473. Membrane fusion mediated intracellular delivery of lipid bilayer coated mesoporous silica nanoparticles. **A. Kros**

11:30 COLL 474. Mechanisms of broad-spectrum antiviral activities of membrane-active molecules targeting enveloped viruses. **A.N. Parikh**

Section D
Ernest N. Morial Convention Center
R06

Chemistry of Molecular Electronics

Monolayers: Tunneling & Function

Cosponsored by PHYS
M.S. Inkpen, G.C. Solomon, L. Venkataraman, *Organizers, Presiding*

8:30 COLL 475. Extracting quantitative information from molecular junction i-v characteristics using a compact analytical model. **C. Frisbie**

9:00 COLL 476. Impact of fluorinated alkanethiols with embedded dipoles on transport properties of EGaIn top contact devices and organic transistors. **R.C. Bruce**, L. You, L.A. Fredin, A. Förster, E. Bittle, D. Vang, S. Pookpanratana, O. Pomerenk, C.A. Hacker

9:20 COLL 477. Single-molecule conductance measurements in solutions and self-assembled monolayers. **M.S. Inkpen**, Z. Liu, H. Li, L.M. Campos, J. Neaton, L. Venkataraman

9:40 COLL 478. Electrostatic vs. quantum-mechanical coupling in self-assembled monolayers and its impact on ballistic transport through self-assembled monolayers. **E. Zojer**

10:10 Intermission.

10:20 COLL 479. Synthesis and self-assembly in tunneling junctions comprising molecular switches. **R.C. Chiechi**, S. Kumar, J. van Herpt, R. Gengler, B. Feringa, P. Rudolf

10:50 COLL 480. Superexchange tunneling: A lesson from nature. **M. Baghbanzadeh**, C.M. Bowers, D. Rappoport, L. Yuan, T. Zaba, P. Cyganik, A. Aspuru-Guzik, G.M. Whitesides

11:10 COLL 481. Effect of heteroatom substitution on transport in alkane dithiol based molecular tunnel junctions: Evidence for universal behavior. **Z. Xie**, I. Baldea, C. Frisbie

11:30 COLL 482. Transition from direct to inverted charge transport Marcus regions in molecular junctions via molecular orbital gating. **E. del Barco**, Y. Li, L. Wang, A. Rodriguez, M. Anguera Antonana, H. Venkata Annadata, C.A. Nijhuis

11:50 COLL 483. Directional plasmon launching from large-area molecular tunnelling junctions. **C.A. Nijhuis**

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
F. Bai, H. Fan, Y. Han, *Organizers*
M. Cai, *Organizer, Presiding*
H. Fan, *Presiding*

8:30 COLL 484. Engineering colloidal semiconducting heteronanorods for solar energy conversion. **S. Yu**

9:00 COLL 485. Direct imaging of single nanoparticle reaction dynamics using *in-situ* liquid cell electron microscopy. **X. Ye**

9:30 COLL 486. Shape-changing and motile colloidal assemblies: Sequence-encoded microbots and colloidal origami from patchy magnetic cubes. **O.D. Velev**, K. Han, C. Shields, G.P. López

9:50 COLL 487. Self-organization of silica colloidal particles confined in water-in-oil droplets. **W. Sun**, S. Chen, M. Xu, Y. Wei, T. Fan, G. Yuan

10:10 Intermission.

10:30 COLL 488. Silicon nanocrystals. **B.A. Korgel**

11:00 COLL 489. Ultra-photostable lead chalcogenide giant quantum dots: A case study in materials-by-design. **J.A. Hollingsworth**, H. Htoon, C. Hanson, A. Singh, S. Krishnamurthy, Z. Hu, A.E. King, A. Piryatinski

11:30 COLL 490. Tunable amorphous photonic materials with pigmentary colloidal nanostructures. **Y. Han**, J. Han, E. Lee, A. Pascall, J. Kuntz, M.A. Worsley

11:50 COLL 491. Withdrawn

12:10 COLL 492. Direct assembly of nanoparticle arrays by electrophoretic deposition. **P. Mulvaney**

Section F
Ernest N. Morial Convention Center
R09

Solubility of Colloids in Different Solvents

N. Feliu, *Organizer*
L. Liz Marzan, W. Parak, *Organizers, Presiding*

8:30 COLL 493. Designing nanoparticles for ultrasensitive biosensing. **M. Stevens**

8:55 COLL 494. Sedimentation of nanocrystals in different solvents studied by analytical ultracentrifugation. **P. Mulvaney**

9:20 COLL 495. Gold nanorods: Can we still do better? **L. Liz Marzan**

9:45 COLL 496. Tableting nanoparticle reagents to simplify diagnostic processes. **W. Chan**

10:10 COLL 497. Synergizing nanoproperties for effective cancer nanomedicine. **Y. Shen**

10:35 COLL 498. Scanning probe block copolymer lithography as a route to combinatorial nanoscience. **C.A. Mirkin**

11:00 COLL 499. Hedgehog particles. **N. Kotov**

11:25 COLL 500. Solvent-induced reversible self-organization of plasmonic nanoparticles in confined spaces. **M. Grzelczak**, A. Sanchez-Iglesias, N. Claes, S. Bals, L. Liz Marzan

11:50 COLL 501. Multiplex functions of DNA functionalized gold nanoparticles. M. Kyriazi, A. El-Sagheer, T. Brown, O. Muskens, **A. Kanaras**

12:15 COLL 502. Controllable hydrophobicity of gold nanoparticles coated with 18-CROWN-6-C-SH. **A.P. Hill**, M. Brust

Section G
Ernest N. Morial Convention Center
Room 203

Nanomaterials

Novel Synthesis & Nanostructures

J.A. Hollingsworth, R. Nagarajan, *Organizers*
A.B. Greytak, *Presiding*

8:30 COLL 503. Experimental and computational development of single source precursors to Sn-Ge nanocrystals. **J. Vela**, M.A. White, H. Andaraarachchi

9:00 COLL 504. Phase control in the synthesis of metal sulfide nanocrystals. **J. Macdonald**, J. Rhodes, A.D. Leach

9:30 COLL 505. Multicomponent hollow transition metal oxide nanoparticles: Structure-property correlation. **E. Shevchenko**

10:00 COLL 506. Hierarchical chirality in inorganic nanocrystals and their superstructures. **P. Wang**, S. Yu, M. Ouyang

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10:20 COLL 507. Chemically tunable 2-dimensional layered silicon telluride, Si_2Te_3. **K.J. Koski**

10:40 COLL 508. Modeling the growth of transition metal dichalcogenide. **H. Chan**, M. Cherukara, B. Narayanan, S. Sankaranarayanan

11:00 COLL 509. Precise size control of $CsPbX_3$ perovskite quantum dots via thermodynamically controlled synthesis. Y. Dong, T. Qiao, **D.H. Son**

11:20 COLL 510. Blue electrogenerated chemiluminescene from halide perovskite nanocrystals. **Y. Wusimanjiang**, V. Arau, J. Yadav, S. Pan

11:40 COLL 511. Wafer scale synthesis of semiconducting SnO monolayers from interfacial oxide layers of metallic liquid tin. **T. Daeneke**, R.B. Kaner, K. Kalantar-zadeh

Section H
Ernest N. Morial Convention Center
Room 204

Recent Advances in Particulate & Colloid Materials for Biomedical Applications

M.A. Quadir, *Organizer*
B. Rasulev, A.S. Voronov, *Organizers, Presiding*

8:30 COLL 512. Iron oxide nanoparticle clustering increases drug uptake and release. P. Price, K. Carlson, J. Dittmar, A. Kohut, A. Voronov, **L. Bronstein**

8:55 COLL 513. Recent advances in the use of colloidal Gold nanoparticles in cancer therapy. **D. Chithrani**

9:20 COLL 514. Multiple therapeutic objectives from single colloidal assemblies. **G.D. Bothun**

9:45 COLL 515. Clay nanotube biocomposites: Sustained drug delivery and tissue scaffolds. **Y.M. Lvov**

10:10 Intermission.

10:25 COLL 516. Thermal stabilization of enzymes with biocompatible stiff polymer brush ligands. **S. Minko**

10:50 COLL 517. Stimuli-sensitive polymersomes for drug delivery to solid tumors. **S. Mallik**, P. Kulkarni, F. Karandish, M. Confeld

11:15 COLL 518. Hybrid nanoparticles as an alternative to conventional antibiotics. **G. Ferreres Cabanes**, A. Bassegoda, T. Tzanov

11:35 COLL 519. Nanosubstrate-mediated intracellular delivery for high-throughput gene modification. **N. Wattanatorn**, S. Hou, Q. Yang, C. Zhao, X. Xu, H. Tseng, S. Jonas, P.S. Weiss

11:55 COLL 520. Hybrid nanoantibacterials for controlling bacterial infections and spread of drug resistance. **K. Ivanova**, J. Hoyo, A. Ivanova, S. Perez Rafael, T. Tzanov

Section I
Ernest N. Morial Convention Center
Room 205

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Atomic-Layer Deposition & its Applications

Cosponsored by WCC
H. Lee, *Organizer*
A.V. Teplyakov, *Organizer, Presiding*

8:30 COLL 521. New approaches for area-selective atomic layer deposition of oxides. **A. Mackus**

9:00 COLL 522. Approaches to atomic-scale engineering through selective processes. **K. Nardi**, N. Draeger, D. Hausmann, D. Smith

9:30 COLL 523. Gas phase routes to solid catalyst materials. **P.C. Stair**

10:00 COLL 524. Challenges for selective atomic layer deposition. **Y.J. Chabal**, R. Rahman, J. Klesko, A. Dangerfield

10:30 Intermission.

10:45 COLL 525. Adsorption calorimetry during atomic-layer deposition (ALD) and when growing model catalysts. **C.T. Campbell**

11:15 COLL 526. Zintl template formation and function during atomic layer deposition growth of crystalline perovskites on Ge (001) and crystalline oxides on GaN(0001). **J.G. Ekerdt**

11:45 COLL 527. Atomic layer deposition on T-shirts. **H. Lee**

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, ENVR‡, INOR, PMSE‡ and PRES‡

Physical Chemistry of Ionic Liquids

Computation, Theory & Simulation

Sponsored by PHYS, Cosponsored by COLL‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 242

ACS Award Lectures
Cosponsored by CATL‡
R. Nagarajan, *Organizer*
E. Borguet, *Presiding*

2:00 Introduction of Awardee.

2:10 COLL 528. Award Address
(ACS Award in Colloid Chemistry
Sponsored by the Colgate-Palmolive Company). Colloidal stability in the living cell. **H. Wennerström**, M. Oliveberg, E. Vallina, J. Danielsson

3:00 Introduction of Awardee.

3:10 COLL 529. Award Address
(ACS Award in Surface Chemistry
Sponsored by the ACS Division of Colloid and Surface Chemistry). Molecular functionalization of surfaces: An evolution from fundamentals to applications. **S.F. Bent**

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, INOR, PHYS‡, PMSE‡ and PRES‡

WCC Rising Star Award Symposium
Sponsored by WCC, Cosponsored by BIOT, CHED, COLL, INOR and PROF

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Functional Structures from Wood-Based Materials

Fibers & Filaments

Sponsored by CELL, Cosponsored by COLL

Adaptive Nanogels
Sponsored by POLY, Cosponsored by COLL

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY EVENING

Adaptive Nanogels
Sponsored by POLY, Cosponsored by COLL

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 242

Basic Research in Colloids, Surfactants & Nanomaterials

Colloids

R. Nagarajan, *Organizer*
B. Bharti, *Presiding*

8:30 COLL 530. Long-range electrostatic forces in ionic liquids. **H.A. Dobbs**, M.A. Gebbie, M. Valtiner, X. Banquy, Z. Berkson, G. Degen, K. Kristiansen, **J.N. Israelachvili**

8:50 COLL 531. Understanding network formation and strength development in alkali-activated aluminosilica cements. **Z. Berkson**, H.A. Dobbs, K. Kristiansen, G. Degen, B. Chmelka, J.N. Israelachvili

9:10 COLL 532. From plants to clouds – how nanostructured materials mediate transport and phase behavior of water in the environment. **A. Stroock**, A. Robin, P. Lidon, O. Vincent, H. Lu

9:30 COLL 533. Investigating mono- and divalent cation induced aggregation of gold nanoparticles in aqueous environments via surface-enhanced Raman spectroscopy. **M. Chan**, W. Leng, P.J. Vikesland

9:50 COLL 534. Programming non-linear active motion of colloids by designing surface force distribution. J. Lee, **B. Bharti**

10:10 COLL 535. Giant non-aqueous Pickering bubbles: effect of nanoparticle diameter and morphology on stability. **M. Rymaruk**, S.P. Armes, E. Wanless, C. Williams, S. Brown

10:30 COLL 536. Computational approach to evaluation of Hamaker constants. **K. Hongo**, R. Maezono

10:50 COLL 537. Colloidal stabilization of silica and iron oxide nanoparticles in highly concentrated divalent salts. **C. Dandamudi**, G. Beniah, J. Lee, B.A. Lyon, J. Han, K.D. Pennell, N.A. Lynd, K.P. Johnston

11:10 COLL 538. Nanocellular foaming of PLLA spherulites in supercritical CO_2: Control of cell morphology by spherulitic structure. **J. Li**, X. Liao, J. Yang, Q. Jiang, G. Li

11:30 COLL 539. Effect of cellulosic fibers on foam dynamics. **W. Xiang**, N. Preisig, C. Stubenrauch, B.L. Tardy, C. Laine, T. Hjelt, T. Tammelin, J. Ketoja, O. Rojas

11:50 COLL 540. Composition change at the stern layer of the electrolyte-silica interface leads to false potentiometric titration interpretation of surface charge density. **A. Goel**, M.A. Brown

12:10 COLL 541. Numerical study of the dynamics of oil-in-water droplet formation in a coaxial micro-channel. **C. Deng**, **H. Wang**, **W. Huang**

Section B
Ernest N. Morial Convention Center
Room 245

Biomaterials & Biointerfaces

Interactions of Biomolecules & Lipids

V. Gordon, *Organizer*
A.P. Goodwin, *Organizer, Presiding*

8:30 COLL 542. Probing nanolipoprotein particle interactions with supported lipid bilayers at the nanoscale. **A.T. Dang**, M. Coleman, T. Kuhl

8:50 COLL 543. Stimulatory effect of phosphatidylglycerol micelle tubes on β-synuclein aggregation. Z. Jiang, J.D. Flynn, **J.C. Lee**

9:10 COLL 544. Signal transduction on membrane surfaces. **J.T. Groves**

9:40 COLL 545. Interactions of phospholipids and proteins dictate

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vaporization of fluorocarbon droplets for ultrasound imaging. R. Chattaraj, **A.P. Goodwin**

10:10 Intermission.

10:30 COLL 546. Janus particles induce defects in supported lipid bilayers. **K. Lee**, Y. Yu

10:50 COLL 547. Integration of biomembrane in synthetic nanoparticle for diagnosis and therapy. **S. Aryal**, T. Nguyen, A. Pitchaimani

11:20 COLL 548. Characterization of the binding of vesicles, viruses and cells to biomimetic lipid bilayers. **M. Verheijden**, D. Di Iorio, G. Koçer, J. Huskens, P. Jonkheijm

11:40 COLL 549. Nanoscopic rotational tracking reveals binding dynamics of cell membrane-camouflaged nanoparticles on lipid membranes. **Y. Yu**, Y. Gao, Y. Yu

12:00 COLL 550. Attachment of *Alcanivorax borkumensis* to oil-in-water emulsion droplets stabilized by different dispersants. **A. Abbasi**, G.D. Bothun, A. Bose

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, A.N. Parikh, *Organizers*
M. Nieh, *Organizer, Presiding*
J. Nickels, A. Vaish, *Presiding*

8:30 COLL 551. GPCR ligand residence times obtained by all-atom simulation. **L. Chen**, E. Lyman

8:50 COLL 552. Multi-component lipid bilayer membranes on GO: Domain distribution and fluidity evaluation. **R. Tero**, Y. Okomoto, S. Saito

9:20 COLL 553. *In-vivo* structure of the Gram-positive bacterial plasma membrane. **R.F. Standaert**

9:50 COLL 554. Molecular modeling of nanoparticle permeation in lipid membranes for drug delivery applications. P. Oroskar, C. Jameson, **S. Murad**

10:20 COLL 555. Effects of incorporating channel forming peptides on the thermal fluctuations in lipid bilayers. **M. Nagao**, E.G. Kelley, P. Butler

10:50 COLL 556. GPCR-chol interactions: Predictions from all-atom and coarse-grained simulations. **E. Lyman**, L. Yang, E. Rouviere, C. McGraw, A.S. Robinson

11:20 COLL 557. Composition and physical properties of living membranes. **I. Levental**, J. Lorent, K. Levental

11:50 COLL 558. Structural basis of hydrophilic-polymer-modified lipid domains in supported lipid bilayer and their physical properties. **Y. Kakimoto**, R. Tero

12:10 COLL 559. QCM-D study of formation of five-component supported lipid bilayer incorporating cholesterol, sphingomyelin, and ganglioside. **E. Kamaloo**, R. Nagarajan, T.A. Camesano

Section D
Ernest N. Morial Convention Center
R06

Fundamentals & Applications of Emulsions at Nonstandard Conditions

L. Chen, H. Katepalli, R. Moglia, *Organizers, Presiding*

8:30 COLL 560. Coalescence and spontaneous emulsification in the presence of asphaltenes. **G.G. Fuller**, S. Bochner, M. Merola, D. Vlassopoulos

9:10 COLL 561. Non-aqueous emulsion as a versatile tool for new types of nanoparticles. **M. Klapper**, F. Karagoez, D. Vidakovic, K. Muellen

9:35 COLL 562. Microtensiometer platorm for characterization of fluid-fluid interfaces through sudden changes in environment. **L. Walker**

10:00 COLL 563. Hollow microspheres using interfacial trapping of pristine graphene sheets. **C.D. Liyanage**, D.H. Adamson

10:25 COLL 564. Exopolymer produced in the marine environment enhances the stability of oil in water emulsions under saline conditions. **M. Omarova**, L.T. Swientoniewski, I. Mkam Tsengam, D.A. Blake, A. Panchal, Y.M. Lvov, T. Yu, D. Zhang, V.T. John

10:50 COLL 565. Development, characterization, and application of novel high temperature thermoplastic and thermoset dispersions. **D. Dermody**, D. Malotky, R. Lundgard, R. Moglia, M. Sekharan, M. Kalinowski, T. Young, J. Romick, D. Himmelberger, J. Mecca

11:15 COLL 566. High pressure CO_2-in-mineral oil emulsions and N_2-in-mineral oil foams stabilized by polydimethylsiloxane-based surfactants as a waterless hydraulic fracturing fluid. **S. Alzobaidi**, J. Lee, C. Da, G. Rodriguez, J. Harris, R.J. Perry, K.P. Johnston, R.M. Enick

11:40 COLL 567. Schizophrenic diblock copolymer functionalized nanoparticles as temperature responsive Pickering emulsifiers. **H. Katepalli**, M. Ranka, D. Blankschtein, T. Hatton

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
M. Cai, H. Fan, Y. Han, *Organizers*
F. Bai, *Organizer, Presiding*
Y. Jiang, *Presiding*

8:30 COLL 568. Structure influence on the mechanical properties of self-assembled nanoparticle systems. **X. Lin**

9:00 COLL 569. Novel approaches to nanoparticle size control through continuous growth. **D. Huber**

9:30 COLL 570. Epitaxially grown particle superlattices via DNA-programmed assembly on lithographic templates. **R. Macfarlane**

9:50 COLL 571. Pd-decorated Au nanorods via biomimetic techniques for use as plasmonic catalysts in Suzuki coupling of aryl chlorides. **B. Briggs**, M. Smith, J. Wagner

10:10 Intermission.

10:30 COLL 572. Developing hierarchical hybrid polymer-enzyme structures for biomass conversions. **T. Li**, G. Babnigg, J. Johnson

11:00 COLL 573. Liquid evaporation-driven assembly of 3-D architected structures by low-dimensional deformable nanomaterials. **B. Xu**

11:30 COLL 574. Atomistic modeling of nanoparticle self-assembly: dynamics, interactions and structures. **P. Kral**

11:50 COLL 575. Kinetic treatment of the metal-ligand binding for predictive synthesis of colloidal nanoparticles. **S. Mozaffari**, W. Li, C. Thompson, S. Ivanov, A.M. Karim

12:10 COLL 576. Investigation of conduction electrons wave function delocalization at the metal nanoparticle–organic ligand interface in solid state. **T. Habarakada Liyanage**, R. Sardar

Section F
Ernest N. Morial Convention Center
R09

Solubility of Colloids in Different Solvents

L. Liz Marzan, *Organizer*
N. Feliu, W. Parak, *Organizers, Presiding*

8:30 COLL 577. Solubility adjustment of nanocrystals for their use in nanocomposites and in biological environment. **H. Weller**

8:55 COLL 578. Optimized multifunctional polymer coating for tuning nanocrystal solubility. W. Wang, Z. Ji, A. Kapur, **H.M. Mattoussi**

9:20 COLL 579. Directing gold nanoparticles into biological membranes by fine tuning their dispersibility. **M. Brust**

9:45 COLL 580. Surface-Enhanced Raman Scattering (SERS) classification of *K-Ras* point mutations. **L. Guerrini**

10:10 COLL 581. Understanding the interaction of nanoparticles and cells: Potential cytotoxicity associated with the uptake of nanoparticles by cells. **N. Feliu**, W. Parak

10:35 COLL 582. Degradation of particles effects their colloidal properties. **W. Parak**

11:00 COLL 583. Microfluidics and metabolic dying in liquid biopsy. **R.A. Alvarez-Puebla**

11:25 COLL 584. Molybdenum disulfide (MoS_2)/graphene oxide (GO) nanocomposites show favorable lung targeting and enhanced drug loading/tumor-killing efficacy with desirable biocompatibility. **S. Liu**

11:50 COLL 585. Beauty of metal-organic framework bulk chemistry combined with the fascinating world of nanoparticles. **S. Wuttke**

12:15 COLL 586. Coordinating polymer with multiple phosphonic acid anchors for surface-functionalizing metal and metal-oxide nanoparticles. **L. Du**, W. Wang, G. Palui, H.M. Mattoussi

12:35 COLL 587. Photo-promoted ligand exchange of gold colloids with lipoic acid-based polymers. **Z. Jin**, Y. Sugiyama, **C. Zhang**, G. Palui, L. Du, H.M. Mattoussi

Section G
Ernest N. Morial Convention Center
Room 203

Nanomaterials

Nanocomposite Applications: From Plasmonics & Electronics to Biology

J.A. Hollingsworth, R. Nagarajan, *Organizers*
G. Davies, *Presiding*

8:30 COLL 588. Nanostructured plasmonic surfaces for diagnostics and chemistry. **H. Moehwald**, G. Zhang

8:50 COLL 589. Monitoring plasmonic photocatalysis at the single molecule level with surface-enhanced Raman spectroscopy. **J.L. Brooks**, R.R. Frontiera

9:10 COLL 590. Colloidal, nanoelectronic state machines based on 2D materials for aerosolizable electronics. **V. Koman**, P. Liu, D. Kozawa, A. Liu, A. Cottrill, M. Strano

9:30 COLL 591. Effect of particle distance in magnetic properties of superparamagnetic iron oxide nanoparticle and its application in contrast enhance magnetic resonance imaging. **T. Nguyen**, A. Pitchaimani, C. Ferrel, S. Aryal

9:50 COLL 592. Electrical conductivity and Seebeck coefficient of air-stable n-type polymer composite films. **T. Sutch**, J. Allred, G. Szulczewski

10:10 COLL 593. Highly tunable platform for biomimetic catalysts from nanocrystal-polymer composites. **A. Riscoe**, C. Wrasman, A. Menon, M. Hubert, A. Dai, M. Vargas, E. Goodman, A. Yang, A. Beck, L. Wu, M. Cargnello

10:30 COLL 594. Local-mapping and photothermal tumor treatment using galectin-1 targeting nanomaterials. **S.V. Jenkins**, R.P. Dings, J. Chen, R.J. Griffin

10:50 COLL 595. Selenium-containing polymer@metal-organic frameworks nanocomposites as an efficient multi-responsive drug delivery system. **W. Zhou**, W. Zhang, W. Huang, F. Huo

11:10 COLL 596. Macromolecularly "caged" carbon nanoparticles for intracellular trafficking via switchable photoluminescence. **I. Srivastava**, S.K. Misra, I. Tripathi, E. Daza, F. Ostadhossein, D. Pan

11:30 COLL 597. Ultrasound and enzymes for surface functionalization of medical textiles and devices with antimicrobial nanoparticles. **T. Tzanov**, K. Ivanova

Section H
Ernest N. Morial Convention Center

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Room 204

Recent Advances in Particulate & Colloid Materials for Biomedical Applications

A.S. Voronov, *Organizer*
M.A. Quadir, B. Rasulev, *Organizers, Presiding*

8:30 COLL 598. Self-dispersing and stimuli-responsive polyurethane dispersions. H. Gupta, **J. Texter**

8:55 COLL 599. Synthesis and cell attachment study of hybrid molecular brushes with chitosan backbone as potential materials for wound healing. M. Chawathe, S. Jonnalagadda, **A. Sidorenko**

9:20 COLL 600. Surface chemistry modulation in layer-by-layer nanoparticles: How the outer layer dictates nanoparticle-cell interactions. **S. Correa**, E.C. Dreaden, A. Barberio, M.A. Quadir, P.T. Hammond

9:45 COLL 601. Mesoporous nanoparticle-supported hybrid bilayers for drug delivery. **S. Shin**, H. Monteith, W. Paxton

10:10 Intermission.

10:25 COLL 602. Atomistic modeling of nanoparticles engineered for bio-applications. **P. Kral**

10:50 COLL 603. Quantum chemical study on binding of selected amino acids with graphene. **T. Dinadayalane**, D.A. Daggag, J. Lazare, T. Dorlus

11:15 COLL 604. Controlled surface modifications of polyester fibers by using Hansen solubility parameters. **G. Sun**, M. Tamizifar

11:40 COLL 605. Janus nanoparticles for T-cell activation: Clustering ligands to enhance stimulation. **K. Lee**, Y. Yu

12:05 COLL 606. Multifunctional perflurocarbon nanoparticles for targeting and imaging of lung cancer. **L. Wu**, M. Shao, R. Zhang, H. Wang, X. li, Y. Li, X. Xu, H. Zou, G. Lanza, B. Shen

Section I
Ernest N. Morial Convention Center
Room 205

Surface Chemistry

Polymers & Hydrophobic Surfaces

S.L. Tait, *Organizer*
J. Ngunjiri, C. Rosu, *Presiding*

8:30 COLL 607. Variable lysozyme transport dynamics on oxidatively functionalized polystyrene films. **N. Moringo**, H. Shen, L. Tauzin, W. Wang, L. Bishop, C.F. Landes

8:50 COLL 608. Biomimetic water-repellent polyester fabrics with long-time durability and mechanical robustness. **C. Rosu**, V. Breedveld, D.W. Hess

9:10 COLL 609. Migration of erucamide in polyethylene films at elevated temperatures. **J. Ngunjiri**, M.L. Pacholski, K. Laughlin, R. Sharma, V. Kalihari, M. Kapur

9:40 COLL 610. Wrinkled polymer interfaces: Tuning morphologies in ultrathin polymer brush surfaces via postpolymerization modification and soft lithography techniques. **C. Reese**, B. Thompson, P. Logan, D.L. Patton

10:00 Intermission.

10:20 COLL 611. Facile approach to large-scale and three-dimensional pore-forming on polymeric objects. **W. Sun**, J. Zhu, Z. Yin

10:40 COLL 612. Polymer CORALs with single and double response. Z. Friar, P.B. Moore, **A. Sidorenko**

11:10 COLL 613. Materials for moisture harvesting above dew point temperature. **J. Song**, K. Yeung

11:30 COLL 614. Surface plasmon & visible light for polymer functionalization of mesoporous silica films. **N. Herzog**, A. Andrieu-Brunsen

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Kinetics

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Functional Structures from Wood-Based Materials

Paper & Fibrils

Sponsored by CELL, Cosponsored by COLL

Physical Chemistry of Ionic Liquids

Structure

Sponsored by PHYS, Cosponsored by COLL‡

Biobased Gels & Porous Materials

Functionalised Nanocellulose Gels

Sponsored by CELL, Cosponsored by COLL and PMSE

Adaptive Nanogels
Sponsored by POLY, Cosponsored by COLL

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 242

Basic Research in Colloids, Surfactants & Nanomaterials

Applications

R. Nagarajan, *Organizer*
M.A. Ilies, *Presiding*

2:00 COLL 615. Multifunctional carbon dots for tracking and eradication of drug resistant superbugs. **P.C. Ray**

2:20 COLL 616. Electrostatic stabilization of NanoRDX. **M. Doukkali**, R. Patel, V. Stepanov, H. Hadim

2:40 COLL 617. Machine learning to better understand hard surface cleaning formulations. **N.S. Brown**, A. Ryan

3:00 COLL 618. Advancements in latent fingerprint development. P. Villarreal, I. Villavicencio, **S. Liu**, J.L. Liu

3:20 COLL 619. Langmuir films of layered materials: Towards large-area devices. **M. Large**, S. Ogilvie, C.L. Lee, G. Fratta, A.A. King, A. Dalton

3:40 COLL 620. Efficient and synergistic nucleic acid delivery with synthetic systems based on pyridinium amphiphiles. **M.A. Ilies**, V.D. Sharma, A. Kizewski, U. Satyal

4:00 COLL 621. Novel nanomaterials for water purification: Synthesis, characterization and application of functionalized SWCNTs. **A. Sahu**, K. Blackburn, M. Qumhiyeh, K. Durkin, J.C. Poler

4:20 COLL 622. Role of polymers on fragrance retention, release and sensory perception from surfactant-rich rinse-off cosmetics. **M.S. Vethamuthu**

4:40 COLL 623. Two-dimensional sheet stabilized emulsion based inks. **F. Chen**, D.H. Adamson

5:00 COLL 624. Functionalization of graphene materials for corrosion protection in 2K epoxy and urethane coating systems. **M. Wunch**, S. Mahmood, D. Yang

5:20 COLL 625. Sacha inchi (*Plukenetia volubilis*) oil loaded chitosan-alginate micro/nanoemulsion with antioxidant activity. M. Elgegren, D. Cordova, **S. Kim**, J. Nakamatsu, C. Silva, A. Cavaco-Paulo

Section B
Ernest N. Morial Convention Center
Room 245

Biomaterials & Biointerfaces

Biomolecular Adhesion to Surfaces

V. Gordon, *Organizer*
A.P. Goodwin, *Organizer, Presiding*

2:00 COLL 626. Exploring the influence of amino acid strucutre on interactions between peptides and hematite surfaces. **J.A. Dunn**, N.N. Casillas Ituarte, S. Lower, B.H. Lower

2:20 COLL 627. Forthcoming renaissance for calcium phosphate nanoparticles in biomedicine. **V. Uskokovic**

2:40 COLL 628. Sunblock based on bioadhesive nanoparticles. **Y. Deng**

3:00 COLL 629. Enhanced stability of immobilized enzymes on heterogeneous lipid bilayers. **A.F. Chaparro Sosa**, D.F. Kienle, R. Falatach, J. Kaar, D.K. Schwartz

3:20 Intermission.

3:40 COLL 630. Solution-phase zwitterionic polymers destabilize proteins compared to polyethylene glycol. **L. Kisley**, M. Gruebele, D.E. Leckband

4:00 COLL 631. Biointerfacial phenomena in mussel-inspired polymers. P. Delparastan, K. Malollari, **P.B. Messersmith**

4:30 COLL 632. Connecting protein structure, function, and interfacial dynamics with single-molecule methods. **J. Kaar**

5:00 COLL 633. Direct measurements of protein folding stability in biomaterials. **D.E. Leckband**, L. Kisley, K.A. Serrano, D. Guin, X. Kong, M. Gruebele

5:30 COLL 634. Protein-protein interactions control aggregation at silicone oil-water interfaces. **L. Sorret**, M.A. DeWinter, D.K. Schwartz, T. Randolph

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

S. Muralidharan, M. Nieh, A.N. Parikh, *Organizers*
J. Katsaras, *Organizer, Presiding*
M. Nagao, *Presiding*

2:00 COLL 635. Membrane phase separation enhances liposomal delivery of chemotherapeutics. **Z. Imam**, M. Mendicino, J. Stachowiak

2:20 COLL 636. Intrinsically disordered proteins sense membrane curvature. **W. Zeno**, U. Baul, W. Snead, L. Wang, E.M. Lafer, D. Thirumalai, J. Stachowiak

2:50 COLL 637. Building the tight junction: Probing the assembly and regulation of membrane interface organization through *in vitro* reconstitution. **B. Belardi**, T. Hamkins-Indik, D.A. Fletcher

3:20 COLL 638. Non-equilibrium shape transitions of vesicles under osmopheretic flow and its role in biology. **S. Purushothaman**, **S. Emami**, **D. Chang**, **A.N. Parikh**

3:50 COLL 639. Chemoselective construction of biomimetic membranes. **R.J. Brea Fernández**, N.K. Devaraj

4:20 COLL 640. Elucidating the fundamental mechanisms of surfactant-membrane interactions. **L.S. Small**, J. Churchwell, E. Eis, M. Staykova, C.D. Bain

4:50 COLL 641. Dynamic profiling of lipid molecules at picosecond time scale. **D. Bolmatov**, M. Zhernenkov

Section D
Ernest N. Morial Convention Center
R06

Sol-Gel in Nanotechnology: Theory, Synthesis, Characterization & Applications

B.P. Chauhan, *Organizer, Presiding*

2:00 COLL 642. Polyimide aerogel coatings for carbon nanotube wire insulation. **H. Guo**, O. Dewey, M. Meador, L.S. McCorkle, M. Pasquali

2:30 COLL 643. Scaffolded nanocomposites of aminosilane-stabilized metal-core nanoparticles and carbon nanotubes. **B.P. Chauhan**, I. Kang, K. Yeh, Q. Johnson

3:00 COLL 644. Predicting surface area in green synthesis of sol-gel materials. **B.K. Peterson**, M. Afeworki, D.C.

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Calabro, Q. Li, S. Weston

3:30 COLL 645. 3D graphene oxide sol-gel assembly: effects of ammonia and nanosheet morphology on gel properties and their use as structural electrodes for energy storage. D. Parviz, **S. Shah**, M.G. Odom, W. Sun, D. Kulhanek, M.J. Green

4:00 COLL 646. Thermoresponsive coatings on mesoporous-shelled hollow particles serve as gates for controlled release. **Y. Su**, V.T. John

4:30 COLL 647. Hint1 regulated self-assembly of nucleoside phosphoramidate functionalized self-assembling peptides. **H. West**, C.M. Csizmar, C.R. Wagner

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
M. Cai, H. Fan, Y. Han, *Organizers*
F. Bai, *Organizer, Presiding*
Y. Jiang, *Presiding*

2:00 COLL 648. Using time-resolved small-angle x-ray scattering to study micellar nucleation during polymerization-induced self-assembly. **M.J. Derry**, O. Mykhaylyk, A. Ryan, S.P. Armes

2:20 COLL 649. Single reagent synthesis of copper sulfide nanoparticles in water. **P. Bergstrom Mann**, S. Fairclough, I. McGregor, M. Ma, G. Hogarth, M. Thanou, N.J. Long, M. Green

2:40 COLL 650. Fabrication of highly ordered polymer-grafted nanorod assemblies. **J. Streit**, K. Park, A. Jawaid, R. Vaia

3:00 COLL 651. Synthesis of stimuli responsive gold nanoclusters via genetically encoded polymers. **Y. Chen**, A. Desireddy, S. Chakraborty, E. Balog, R.C. Rocha, J.S. Martinez

3:20 COLL 652. Graphene-based photonic crystals. **A. Dalton**

3:40 Intermission.

3:50 COLL 653. Development of polyethyleneimine conjugated gold nanoparticles for bio-medical applications: A systematic investigation toward an effective and sustainable approach. **T. Cho**, J.M. Gorham, J.M. Pettibone, J. Liu, J. Tan, V.A. Hackley

4:10 COLL 654. Radial dopant placement with angstom-level control for tuning plasmonic properties in metal oxide nanocrystals. **B. Crockett**, A. Jansons, K.M. Koskela, J.E. Hutchison, D.W. Johnson

4:30 COLL 655. Switchable surfactants for the preparation of monodisperse, sinter-resistant supported nanoparticles. **K. Bryant**

4:50 COLL 656. Tuning gold nanoparticle assemblies with a family of azobenzene peptide conjugates. **Y. Zhou**, A. Merg, N.L. Rosi

5:10 COLL 657. Photoactivated release from polydopamine nanotubes. Y. Sun, **E.W. Davis**

Section F
Ernest N. Morial Convention Center
R09

Basic Research in Colloids, Surfactants & Nanomaterials

Gels & Responsive Colloids

R. Nagarajan, *Organizer*
A.V. Mallia, *Presiding*

2:00 COLL 658. Supermolecular hydrogel prepared form thymine-containing artificial nucleolipid: Study of assembly and lyotropic mesophases. **D. Zhang**

2:20 COLL 659. Self-healing hydrogels: Relation between microscopic dynamics and macroscopic viscoelasticity. **R. Lund**, L. Willner, T. Zinn, O. Holderer

3:00 COLL 660. High-speed AFM reveals detail understanding in adsorption of soft hydrogel microspheres onto solid substrate in aqueous solution. **S. Matsui**, T. Uchihashi, D. Suzuki

3:20 COLL 661. Effect of surface functional groups on electric stimuli-responsive behavior of polyacrylonitrile dispersed colloid. **T. Do**, Y. Ko

3:40 COLL 662. Gelation studies and thixotropic properties of molecular gels based on ammonium alkanoates as low molecular mass gelators. **A.V. Mallia**, B. Matei, F. Sultan

4:00 COLL 663. Advances in stimuli-responsive properties of functional microbial glycolipids. **N. Baccile**

Section G
Ernest N. Morial Convention Center
Room 203

Basic Research in Colloids, Surfactants & Nanomaterials

Nanoparticle Synthesis & Assembly

R. Nagarajan, *Organizer*
M.L. Personick, *Presiding*

2:00 COLL 664. Withdrawn

2:20 COLL 665. *In situ* monitoring of the reactive crystallization of calcium carbonate in multiphase systems. **T.A. Kathyola**, S. Chang, E.A. Willneff, C. Willis, G. Cibin, P. Wilson, A. Kroner, E.J. Shotton, P.J. Dowding, S. Schroeder

2:40 COLL 666. Composition controllable synthesis of PtCu nanodendrites with efficient electrocatalytic activity for methanol oxidation induced by high index surface and electronic interaction. **L. Lu**

3:00 COLL 667. Strong sensitized phosporescence in Mn-doped $CsPbBr_3$ perovskite nanocrystals. **D. Parobek**, D. Son

3:20 COLL 668. Self-assembly of DNA-coated patchy particles from colloidal fusion. **M. He**, Z. Gong, S. Sacanna, D. Pine

3:40 COLL 669. Silica hallow particles prepared by encapsulation of water droplets with perhydropolysilazane in hydrophobic solvents. K. Kuramochi, H. Kiyosawa, **R. Saito**

4:00 COLL 670. Withdrawn

4:20 COLL 671. Hierarchical assembly of supramolecular G-quadruplexes via enzyme instructed self-assembly. **L.A. Prieto-Costas**, J. Rivera, N. Lui

4:40 COLL 672. Coupling competitive surface interactions: A synthetic route to enhanced grain boundaries at the exterior of multiply twinned palladium nanoparticles. **M.E. King**, M.L. Personick

5:00 COLL 673. Pamitoyl-co-enzyme-A colloidal nanoparticles for transcriptional chemo-biologics therapy. **S.K. Misra**

5:20 COLL 674. Rapid fabrication of hollow β-Fe_2O_3 particles with applications to enhanced photo-fenton reactions. **Y. Zhang**, Y. Su, J. He, G. McPherson, V.T. John

Section H
Ernest N. Morial Convention Center
Room 204

Recent Advances in Particulate & Colloid Materials for Biomedical Applications

A.S. Voronov, *Organizer*
M.A. Quadir, B. Rasulev, *Organizers, Presiding*

2:00 COLL 675. Understanding protein uptake properties of ionically crosslinked micro- and nanogels. Y. Cai, **Y. Lapitsky**

2:20 COLL 676. Antibacterial and antibiofilm layer-by-layer decorated nanoparticles. **A. Ivanova**, K. Ivanova, J. Hoyo, T.J. Heinze, T. Tzanov

2:40 COLL 677. Nanoparticle system for pH-triggered aptamer targeting and Pt (II) delivery to cancer cells. M.T. Wlodarczyk, S.A. Dragulska, Y. Chen, O. Camacho-Vanegas, P. Dottino, J.A. Martignetti, **A.J. Mieszawska**

3:00 COLL 678. Stimuli-responsive zwitterionic microgels. **A. Pich**

3:20 COLL 679. Reprogramming growth factor signaling through nanoconjugation. A. Khanehzar, **B.M. Reinhard**

3:40 Intermission.

3:55 COLL 680. Imaging the kinetics of serotonin receptor trafficking with quantum-dot nanoparticles. G.K. Illy, E.B. Nowak, **K. Fichter**

4:15 COLL 681. Nanosized MRI contrast agents: Engineering nanostructure and surfaces for contrast signal control and towards non-invasive diagnostics. **G.H. Lee**, G. Davies, C. Hutchinson

4:35 COLL 682. SERS of bacteria using ag colloid suspensions. **R.D. George**, K. Sorensen, P. Mosier-Boss, P. Sims, A. O'Braztsova

4:55 COLL 683. Indocyanine green-loaded multifunctional multiwalled carbon nanotubes as a versatile platform for targeted dual-mode imaging and phototherapy of tumors. Y. Hu, R. Wang, Y. Zhou, D. Gao, **X. Shi**, M. Shen

5:15 COLL 684. Exploiting Le Chatelier's principle for a one-pot synthesis of nontoxic HHogGNPs with the sharpest nanoscopic features suitable for tunable plasmon spectroscopy and high throughput SERS sensing. **M. Bhattacharya**

Section I
Ernest N. Morial Convention Center
Room 205

Surface Chemistry

Adsorption at Surfaces

S.L. Tait, *Organizer*
C. Carbonell Fernandez, T.J. Mullen, *Presiding*

2:00 COLL 685. Expanding the molecular-ruler process though the solution and vapor deposition of alkanethiol molecules. **T.J. Mullen**

2:30 COLL 686. Reactivity of confined carboxylic acids in thin films. **D.P. Goronzy**, E. Avery, N.M. Gallup, J. Staněk, J. Macháček, T. Baše, K.N. Houk, P.S. Weiss

2:50 COLL 687. Surface-bound SuFEx chemistry: A fast and quantitative organic reaction. D. Gahtory, R. Sen, S.P. Pujari, S. Li, Q. Zheng, J. Moses, K.B. Sharpless, **H. Zuilhof**

3:20 COLL 688. Reactivity, kinetics, and limitations of SuFEx chemistry used for surface functionalization. **K. Brooks**, J. Yatvin, M. Kovaliov, G.H. Crane, S. Averick, J.J. Locklin

3:40 Intermission.

4:00 COLL 689. Multiplexed light-mediated tip-based molecular printing in continuous capillary flow. **C. Carbonell Fernandez**, D.J. Valles, A. Wong, M. Wai, M. Niang, A.B. Braunschweig

4:20 COLL 690. Superamphiphobic wood surfaces. M. Sedighi Moghaddam, M. Tuominen, J. Haapanen, J. Mäkelä, **A. Swerin**

4:50 COLL 691. Dosing drops with liquid needle to measure advancing and static contact angles. **R.J. Sanedrin**, M. Jin, D. Frese, C. Scheithauer, T. Willers

Functional Structures from Wood-Based Materials

Films & Low-Density Composites

Sponsored by CELL, Cosponsored by COLL

Physical Chemistry of Ionic Liquids

Transport & Dynamics

Sponsored by PHYS, Cosponsored by COLL‡

Biobased Gels & Porous Materials

Cellulose & Non-Cellulose Gels: Synthesis, Properties, Applications

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Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

WEDNESDAY EVENING

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 242

Basic Research in Colloids, Surfactants & Nanomaterials

Surfaces & Interfaces

R. Nagarajan, *Organizer*
R. Quinones, *Presiding*

8:30 COLL 692. Low electric and magnetic field induced transient spin dynamics of sanguinarine on single domain nanosurface. **S. Das Chakraborty**

8:50 COLL 693. Chemical mapping of the evolving material interface of particles in liquids. **X. Yu**

9:10 COLL 694. Study of polymorphism using patterned self-assembled monolayers approach on metal substrates. **R. Quinones**

9:30 COLL 695. Balancing multiple orthogonal functions simultaneously on a single surface. **T. Lawton**, J. Uzarski, S. Filocamo

9:50 COLL 696. Controlling surface oxidation of gallium liquid metal colloids through judicious ligand selection. **C.E. Tabor**, Z. Farrell, I. Anderson, C. Thrasher, J. Mingear

10:10 COLL 697. Thermochemical analysis of proton coupled electron transfer at titanium dioxide nanoparticles. **J. Peper**, B. Boudy, J.M. Mayer

10:30 COLL 698. Solvent-dependent ligand structure and conformation on gold and silver nanoparticles. **P.P. De Silva**, D. Zhang

10:50 COLL 699. Surface chemistry of engineered nanoparticles in biological and environmental media of varying pH. **A.H. Alminshid**, V.H. Grassian, S.C. Larsen

11:10 COLL 700. Confocal raman microscopy investigation of mixed-surfactant monolayers at n-alkyl-chain functionalized surfaces in chromatographic particles. **M. Zare**, J.P. Kitt, D. Bryce, J.M. Harris

11:30 COLL 701. Surfactant-free graphene exfoliation study between solvent interfaces. **T. Hui**, D.H. Adamson

11:50 COLL 702. Slippery liquid-immobilized film with high thermal and chemical stability. **S. Shiratori**, Y. Tsuge

Section B
Ernest N. Morial Convention Center
Room 245

Biomaterials & Biointerfaces

Advances in Biomaterials

V. Gordon, *Organizer*
A.P. Goodwin, *Organizer, Presiding*

8:30 COLL 703. Silk fibroin microcapsules as functional bioreactors for *in vitro* protein synthesis. **I. Drachuk**, S. Harbaugh, J.L. Chavez, N. Kelley-Loughnane

8:50 COLL 704. Cellulose biointerface for paper diagnostics. V. Raghuwanshi, Z. Huang, N. Yeow, C. Garvey, R. Tabor, **G. Garnier**

9:10 COLL 705. Surface design of sulfonated-supramolecular substrates for tethering bone morphogenetic protein 2. **Y. Arisaka**, N. Yui

9:30 COLL 706. Blood-vessel-like polymer tubes that can morph their diameter and shape in response to stimuli. **S.R. Raghavan**, B. Zarket

9:50 COLL 707. Rapid electroformation of alginate gels into complex shapes for tissue engineering. **S.R. Raghavan**, A. Gargava

10:10 Intermission.

10:30 COLL 708. Poorly adhesive materials and their affect on cellular metabolism. **R. Surmaitis**, C.J. Arias, J.B. Schlenoff

10:50 COLL 709. Probing forces between stem cells and biomaterials using colloidal probe microscopy. **M.K. Osterberg**, R. Harjumäki, R.W. Nugroho, J. Valle-Delgado

11:10 COLL 710. Nanomaterials for the characterisation of cellular structure and mobility. **A. King**, R. Harries, S. Ogilvie, M. Large, I. Jurewicz, A. Dalton

11:30 COLL 711. Withdrawn

11:50 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
R07

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, M. Nieh, A.N. Parikh, *Organizers*
S. Muralidharan, *Organizer, Presiding*

8:30 COLL 712. Characterizing metallomembranes using vibrational sum frequency spectroscopy. **S. Pullanchery**, S. Sun, M.F. Poyton, P.S. Cremer

8:50 COLL 713. Understanding the permeation of charged peptides through model membranes using experiment and simulation. **C.M. Anderson**, A.E. Cardenas, J. Flanagan, L.J. Webb

9:10 COLL 714. Probing the interaction between antimicrobial peptides and biomembranes using small angle scattering techniques. **J.E. Nielsen**, V. Bjørnestad, R. Lund

9:30 COLL 715. Single molecule detection of biomarker in a nanometric gap structure combined with fluid membrane. **K. Ando**, F. Hayashi, K. Morigaki

9:50 COLL 716. Raftophilicity of membrane proteins in phototransduction evaluated with a micropatterned model membrane. **Y. Tanimoto**, S. Kojima, F. Hayashi, A. Awazu, K. Morigaki

10:10 COLL 717. *In situ* methods for tuning membrane structure and lipid mobility in polyacrylic acid-cushioned supported lipid bilayers. **A.T. Dang**, T. Kuhl

10:30 COLL 718. Withdrawn

10:50 COLL 719. Investigating the dynamics of phosphatidylinositide lipids in supported bilayers. **S. Sun**, D.R. Melendez, C. Liu, T. Yang, P.S. Cremer

11:10 COLL 720. Out-of-plane alignment and in-plane growth of domain in lipid multilayer upon surface ion binding. **S. Lee**, Y. Lee, J. Bak, D. Jeong, J. Lee, H. Lee, C. Hyeon, M. Choi

11:30 COLL 721. Enzymatic strategies of *de novo* phospholipid membrane formation. **A. Bhattacharya**, N.K. Devaraj

11:50 COLL 722. Pulsatile gating of giant vesicles containing macromolecular crowding agents induced by colligative non-ideality. **W. Su**, D.L. Gettel, M. Chabanon, P. Rangamani, A.N. Parikh

Section D
Ernest N. Morial Convention Center
R06

Basic Research in Colloids, Surfactants & Nanomaterials

Interfaces in Amphiphilic Systems

R. Nagarajan, *Organizer*
S. Roke, *Presiding*

8:30 COLL 723. Talking heads: A conversation between co-surfactant head groups at the oil-water interface. **R. Ciszewski**, B. Muller, G.L. Richmond

8:50 COLL 724. New insights on interfacial structure of polymer/surfactant complexes. **B. Schabes**, R. Altman, G.L. Richmond

9:10 COLL 725. Structure-function relationships and worm-like micelle formation of novel carbohydrate-based surfactants. **J. Moore**, C. Garvey, L. de Campo, A. Sokolova, B. Wilkinson, R. Tabor

9:30 COLL 726. Molecule dynamics simulations of the fluorinated and fluorine-free surfactant monolayers at air-water and heptane-water interfaces. **X. Zhuang**, R. Ananth

9:50 COLL 727. Gibbs ensemble Monte Carlo simulations for additive loading in surfactant bilayers. **M.S. Minkara**, J.I. Siepmann

10:10 COLL 728. Zwitterionic and charged lipids form remarkably different structures on nanoscale oil droplets in aqueous solution. Y. Chen, H. Okur, C. Luetgebaucks, **S. Roke**

10:30 COLL 729. Transition of unilamellar cationic liposomes to bilamellar structures through the depletion effect. **Y. Zhang**, J.S. Arora, J. He, V.T. John

10:50 COLL 730. Finding new eco-friendly dispersants for oil-spill remediation: Lignin based solutions for oil-herding. **J. Lee**, J. Cantrell, B. Bharti

11:10 COLL 731. Foam control agent development for food processing. **X. Chen**, S. Ospino, M. Whitley, M. Tulchinsky, W. Gao, T. Zhang, F. Donate, A. Ossola, P. Cameron, B. Radtke, S. King, C. Cummins

11:30 COLL 732. Self-assembled monolayers derived from unsymmetrical spiroalkanedithiols having hydrophobic and hydrophilic tailgroups. **R. Ghanbaripour**, **T. Lee**

11:50 COLL 733. Composition–driven structural transitions from vesicles to bicelles to micells using phospholipid and nonionic surfactant mixtures. **I. Mkam Tsengam**, M. Omarova, S.R. Raghavan, G.D. Bothun, A. Mccormick, V.T. John

Section E
Ernest N. Morial Convention Center
R08

Colloidal Nanoparticle Synthesis & Assembly

Financially supported by Henan University and King Abdullah University of Science and Technology
M. Cai, H. Fan, Y. Han, *Organizers*
F. Bai, *Organizer, Presiding*
Y. Jiang, *Presiding*

8:30 COLL 734. Combination of atomic layer deposition and self-assembly of colloidal nanoparticles for high-performance gas separation membranes. **Y. Jiang**, C. Fan, G. Jiang, Z. Wang, Y. Gao, Y. Tian, H. Zhang

8:50 COLL 735. Phase transferable polymer encapsulated bimetallic nanoparticles. **S. Street**, M. Confer

9:10 COLL 736. Autoperforation of 2D materials for generating two terminal memresistive Janus particles. **A.T. Liu**, P. Liu, M. Strano

9:30 COLL 737. Surface passivation and supersaturation: strategies for regioselective deposition in seeded syntheses. **A. Chen**, M.M. Scanlan, S.E. Skrabalak

9:50 COLL 738. Singly dispersed gold nanoshell-bearing cellulose nanocrystals with tailorable plasmon resonance. **N. Semenikhin**, N. Kadasala, R.J. Moon, J.W. Perry, K.H. Sandhage

10:10 COLL 739. Synthesis of high performance anisotropic $SmCo_5$ nanomagnets by reduction of Co-$Sm(OH)_3$ assembly. **B. Shen**, S. Sun

10:30 COLL 740. Low-temperature solution synthesis of titanium nitride nanoparticles. **A.J. Kuehne**

10:50 COLL 741. Sophorolipid-coated superparamagnetic iron oxide nanoparticles: Synthesis and structure. **A.**

‡*Cooperative Cosponsorship*

Lassenberger, E. Reimhult, N. Baccile

11:10 COLL 742. Alternate path to formation of co-aligned mesocrystals. **G. Zhu**, J.A. Soltis, J. Tao, B. Legg, C. Wang, J. De Yoreo

11:30 COLL 743. Aggregated gold nanoparticles demonstrate increased surface-enhanced Raman scattering activity in presence of hydrogen peroxide. **A.A. Novikov**, M.V. Gorbachevskiy, D.S. Kopitsyn, M.S. Kotelev, Y.M. Lvov, V. Vinokurov

11:50 COLL 744. Approaches for bridging dissimilar reduction kinetics in the synthesis of bimetallic nanomaterials. **M.L. Personick**, A.L. Stone, D. Solti, M.E. King, H. Jung, I.A. Kent

12:10 COLL 745. Self-assembled porphyrin nanocrystals for efficient visible-light-driven hydrogen evolution. **Y. Liu**, F. Bai

Section F
Ernest N. Morial Convention Center
R09

Basic Research in Colloids, Surfactants & Nanomaterials

Biointerfaces

R. Nagarajan, *Organizer*
M.R. Mackiewicz, *Presiding*

8:30 COLL 746. Slippery liquid-infused porous surfaces for cell deformation microfluidic devices and cargo delivery. **A. Mendoza**, C. Zhao, Q. Yang, P. Kim, S. Jonas, P.S. Weiss

8:50 COLL 747. Liquid crystalline particles for delivery of antimicrobial peptides. **L. Boge**, A. Umerska, N. Matougui, H. Bysell, L. Ringstad, M. Davoudi, J. Eriksson, K. Edwards, M. Andersson

9:10 COLL 748. Understanding fine textures in touch — the role of fingerprints in modulating sliding friction on surfaces and haptic devices. **C. Dhong**, D.J. Lipomi

9:30 COLL 749. Versatile glycosurfaces fabrication on poly(pentafluorophenyl acrylate) grafted scaffold via hydrazide conjugation and its application in *Mycoplasma Pneumoniae*. **L. Chen**, C. William, D. Krause, J.J. Locklin

9:50 COLL 750. Covalent grafting of antifouling phosphorylcholine-based copolymers with antimicrobial nitric oxide releasing polymers to enhance infection-resistant properties of medical device coatings. **Q. Liu**, P. Singha, H. Handa, J.J. Locklin

10:10 COLL 751. Cell separation by thermoresponsive nanofibers using N-isopropylacrylamide. **S. Shiratori**, T. Konishi, J. Li, Y. Tokura, M. Tenjimbayashi, K. Homma, K. Matsukawa, A.M. Akimoto

10:30 COLL 752. Interactions of gold nanoparticles and skin. **A. Kanaras**, R. Fernandes

10:50 COLL 753. Nanoparticle-coated surfaces provide quantifiable insight into thermal and radiation effects. **S.V. Jenkins**, R.P. Dings, M. Borrelli, R.J. Griffin

11:10 COLL 754. Nanomaterials for enhancing the resolution of optical coherence tomography in the retina. **M.R. Mackiewicz**, K. Kinnison, J. Stoddard, R.C. Hugo, T.J. McGill

11:30 COLL 755. Antimicrobial amidinourea polymers for treating drug resistance bacteria. M. Ahmed, **J. Moon**

11:50 COLL 756. Dual stimuli platfrom for remotely controlled drug delivery. **A.M. Laradji**, A. Zakharchenko, R. Saremi, N. Yadavalli, A. Gruzd, S. Minko

12:10 COLL 757. Protein-induced gold nanoparticle aggregation probed by label-free second harmonic light scattering. **K. Mishra**, P.K. Das

Section G
Ernest N. Morial Convention Center
Room 203

Basic Research in Colloids, Surfactants & Nanomaterials

Nanomaterials

R. Nagarajan, *Organizer*
P.S. May, *Presiding*

8:30 COLL 758. Unusual p-n heterostructured water-borne nanoparticles exhibiting superior charge separation ability. **Y. Kim**, B. Lee

8:50 COLL 759. Ultrafast dynamics of single aluminum nanostructures. **M. Su**, P.D. Dongare, S.H. Jebeli, D. Renard, Y. Zhang, C. Yi, W. Chang, P.J. Nordlander, N.J. Halas, S. Link

9:10 COLL 760. Fe-l edge spectroscopy reveals the chemistry of iron in nanoscale particulate matter. A. Pattammattel, H. Forman, P.A. O'Day, **V. Leppert**

9:30 COLL 761. Influence of poly-(ethylene glycol) coatings in the surface plasmon resonance induced photothermal property of gold nanorod. **R. Marasini**, A. Pitchaimani, T. Nguyen, S. Aryal

9:50 COLL 762. Beyond the near-field: Enhancing the efficiency of upconversion-luminescence nanomaterials using the diffractive and reflective properties of structured metal surfaces. **P.S. May**, A. Baride, M.T. Berry, S. Smith

10:10 COLL 763. Pressure dependence of excited state dynamics in CdSe/CdS heterostructure nanocrystals. **L. Hanson**, C.W. Li, P. Alivisatos

10:30 COLL 764. Hybrid metal-semiconductor nanoparticles for hot electron luminescence upconversion. **B. Roman**, J. Otto, D. Dacres, C. Galik, R. Downing, M. Sheldon

10:50 COLL 765. Synthesis of Au38(SCH2CH2Ph)24, Au36(SPhtBu)24, and Au30(StBu)18 nanomolecules and structural selectivity. **M. Rambukwella**, A. Dass

11:10 COLL 766. Reactive Ag^{+} adsorption onto gold. **S. Athukorale**, D. Zhang

11:30 COLL 767. Modeling the photon avalanche upconversion mechanism in Tm^{3+}, Yb^{3+} co-doped β-$NaYF_4$ nanocrystals. **M. Hossan**, M. Berry, S. May

11:50 COLL 768. Controlling ligand orientation and conformational order on nanostructured materials. **L.A. Velarde**, S. Sengupta, S.T. Algoul

12:10 COLL 769. Photo-induced electron transfer from amino acids to nitrogen functionalized graphene quantum dots. **S. Mukherjee**, P. Edamana, A. Chadha

Section H
Ernest N. Morial Convention Center
Room 204

Recent Advances in Particulate & Colloid Materials for Biomedical Applications

A.S. Voronov, *Organizer*
M.A. Quadir, B. Rasulev, *Organizers, Presiding*

8:30 COLL 770. Withdrawn

8:50 COLL 771. Active antioxidizing polymeric particles for on-demand pressure-driven molecular release. **Y. Seo**, J. Leong, J. Teo, J.W. Mitchell, M.U. Gillette, B. Han, J. Lee, H. Kong

9:10 COLL 772. $CuInS_2$/ZnS quantum dot based probe for monitoring the acetylation of mitochondrial proteins. **C. Wang**, E. Weiss

9:30 COLL 773. Highly selective capturing of biomolecules by antifouling zwitterionic polymer-coated microbeads. **E. van Andel**, H. Zuilhof, M. Smulders, E. Tijhaar, H. Savelkoul

9:50 COLL 774. Microphysiological multi-tissue platform for simultaneous efficacy and toxicity testing of drug formulations. C. Lohasz, P.M. Misun, F. Bonanini, F. Hürlimann, O. Frey, **K. Renggli**, A. Hierlemann

10:10 Intermission.

10:25 COLL 775. Hybrid nanoparticles of a conjugated polymer and iron oxide nanocrystals for simultaneous photothermal, photoacoustic and magnetic effects. **J. Park**, D. Pham, E. Kang, S. Kim

10:45 COLL 776. Manganoporphyrin-polyphenol multilayer capsules as radical and ROS scavengers. **A. Alford**, V.A. Kozlovskaya, D. Pham-Hua, L. He, V. Urban, H.M. Tse, E.P. Kharlampieva

11:05 COLL 777. Electrically-activated bursting of aqueous microcapsules made from nonconducting, biocompatible polymers: A new mode for drug delivery compatible with wearable electronics. **S.R. Raghavan**, A. Gargava

11:25 COLL 778. Nanoparticle-laden macrophage as a tumor tropic drug delivery system for improved cancer treatment. **W. Zhang**, M. Wang, Z. Zhen, H. Chen, M. Chapman, W. Tang, T. Todd, T. Cowger, S. Zhou, H. Wang, I. Delahunty, Z. Li, J. Xie

11:45 COLL 779. Withdrawn

12:05 COLL 780. Radiofrequency and near-infrared responsive core-shell nanoparticles formed by lipid templating. **A. Pan**, G.D. Bothun

Section I
Ernest N. Morial Convention Center
Room 205

Surface Chemistry

Carbon Surfaces & Environmental Adsorption

S.L. Tait, *Organizer*
L.C. Henderson, L.A. Velarde, *Presiding*

8:30 COLL 781. Modifying the surface of carbon fiber for fiber-to-matrix adhesion. **L.C. Henderson**, L. Servinis, J. Randall, C. Arnold

9:00 COLL 782. Surface modification of sp^2 hybridized carbon nanomaterials via an inverse electron demand Diels-Alder reaction. **J. Zhu**, R. Lennox

9:20 COLL 783. Functionalized carbon nanomaterials for energy storage devices. **J. Zuczek**, N. Elathram, W. Hixson, J.C. Poler

9:40 COLL 784. Composite nanomaterials for water purification: Sustainable high-capacity rapid removal of small molecule DBP precursors. **J.C. Poler**, A. Sahu, K. Durkin, K. Blackburn

10:00 COLL 785. Enhancement of perovskite crystallinity by interfacial lead adsorption on TiO_2. **K.C. Saunders**, J. Stanfill, B. Fessler, R. Shallcross, S.S. Saavedra, N.R. Armstrong

10:20 Intermission.

10:40 COLL 786. Binding and orientation of carbamate pesticides on mineral surfaces. L. Bromley III, J. Cartagena, P. Videla, A. Fernando, V.S. Batista, **L.A. Velarde**

11:00 COLL 787. Revealing the complexities of hydroxyacetone at the air-water via vibrational sum frequency spectroscopy and computational methodologies. **B. Gordon**, F.G. Moore, L.F. Scatena, N.A. Valley, S. Wren, G.L. Richmond

11:20 COLL 788. Native urban films' spatial and chemical heterogeneity reported by microscopy and SIMS analysis. **J.S. Grant**, S.K. Shaw

11:40 COLL 789. Mechanism of adsorption of phosphatidylcholine from a dispersion of vesicles onto a clean air-water interface. **J. Staton**, S.R. Dungan

Elucidation of Mechanisms & Kinetics on Surfaces
Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Functional Structures from Wood-Based Materials

Biosensing & Biomaterials

Sponsored by CELL, Cosponsored by COLL

Physical Chemistry of Ionic Liquids

Interfaces & Ionic Liquid Nanoscience

Sponsored by PHYS, Cosponsored by COLL‡

Biobased Gels & Porous Materials

Biomedical Applications of Polysaccharide Gels & Aerogels

Sponsored by CELL, Cosponsored by COLL and PMSE

‡*Cooperative Cosponsorship*

Adaptive Nanogels
Sponsored by POLY, Cosponsored by COLL

THURSDAY AFTERNOON

Elucidation of Mechanisms & Kinetics on Surfaces
Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Functional Structures from Wood-Based Materials

Designed Structures & Processing

Sponsored by CELL, Cosponsored by COLL

Physical Chemistry of Ionic Liquids

Ionic Liquid-Solute-Solvent Interactions

Sponsored by PHYS, Cosponsored by COLL‡

Adaptive Nanogels
Sponsored by POLY, Cosponsored by COLL

Biobased Gels & Porous Materials

Polysaccharide Foams, Cryogels & Aerogels

Sponsored by CELL, Cosponsored by COLL and PMSE

COMP

Division of Computers in Chemistry

H. Woodcock, J. Shen and M. Feig, *Program Chairs*

SUNDAY MORNING

Section A
New Orleans Marriott Convention Center
New Levee

Molecular Mechanics

Force Fields

M. Feig, *Organizer*
H. Bruce Macdonald, *Presiding*

8:30 COMP 1. Rapid estimation of atomic charges for the first 96 elements. **C.W. Earley**

9:00 COMP 2. Molecular dynamics simulations of ammonia synthesis process on ruthenium nanoparticle catalyst. **S. Kim**, S. Han

9:30 COMP 3. Non-covalent force field expressed in terms of spherical density functions. **T. Verstraelen**, S. Vandenbrande, F. Heidar-Zadeh, L. Vanduyfhuys, M.E. Waroquier, V. Van Speybroeck, P. Ayers

10:00 Intermission.

10:15 COMP 4. Atom in molecules atomic charges based on different partitioning schemes validated for biomolecular free energy calculations. **E. Voehringer-Martinez**, M. Riquelme, A. Lara

10:45 COMP 5. Influence of protein-solvent interactions on the molecular dynamics of reduced point charge models of proteins. **L. Leherte**, D. Vercauteren

11:15 COMP 6. Residue based contributions to the thermodynamic properties of ubiquitin. **N.K. Kariyawasam Manachchige**, E.A. Ploetz, P.E. Smith

Section B
New Orleans Marriott Convention Center
Mississippi Queen

Computational Studies of Water

Models & Biological Applications

D.J. Sindhikara, *Organizer*
H. Torabifard, *Presiding*

8:30 COMP 7. Solvation by single-site multipole water. **T. Ichiye**

9:00 COMP 8. Accurate modeling of water clusters with density-functional theory using atom-centered potentials. **G.A. DiLabio**

9:30 COMP 9. Path integral approach to a strong coupling solution of a coarse grained electronic structure describes water's properties from ice to the supercritical regime. **G.J. Martyna**

10:00 Intermission.

10:15 COMP 10. Computationally efficient approach to estimating the mean solvent density around polar solutes. **M. McCullagh**

10:45 COMP 11. Predicting water networks and ligand binding free energies in proteins using grand canonical Monte Carlo. **H. Bruce Macdonald**, C. Cave-Ayland, J.W. Essex

11:05 COMP 12. Water-multimodal ligand interactions: The effect of ligand chemistry and architecture on ligand hydration and conformation in solution and at interfaces. **C. Bilodeau**, S.M. Cramer, S. Garde

11:25 COMP 13. Characterizing hydration properties based on the orientational structure of interfacial water molecules. **S. Shin**, A.P. Willard

Section C
New Orleans Marriott Convention Center
Julia

Drug Design

Structure & Ligand-Based Design

Cosponsored by CINF
M.R. Landon, Y. Tseng, *Organizers*
P. Buteler, *Presiding*

8:30 COMP 14. *In silico* enzyme engineering: Computational methodology for improving both the catalytic activity and stability. **J. Park**, T. Kim, Y. Choi, Y. Jung, M. Shim, H. Lee

9:00 COMP 15. Dynamic structural differences between human and mouse STING lead to differing sensitivity to DMXAA. **A. Shih**, K. Damm-Ganamet, T. Mirzadegan

9:30 COMP 16. Structure-based optimization of JAK1 ATP-binding pocket inhibitors in the aminopyrazole class. **P.A. Gibbons**, K. Barrett, D. Brown, G. Buckley, G. Hamilton, A. Johnson, T. Kellar, P. Kohli, M. Liimatta, J. Lloyd, A. Romero, G. Salmon, M. Zak, G. Zhao

10:00 Intermission.

10:15 COMP 17. Structural basis of unprecedented potency of GRL-142 against multi-drug resistant HIV-1 protease. **D. Das**, M. Aoki, H. Hayashi, Y. Takamatsu, H. Bulut, R. Yedidi, K.V. Rao, A.K. Ghosh, H. Mitsuya

10:45 COMP 18. Ligand based drug discovery of novel dengue-2 NS2B-NS3 protease inhibitors. **H.A. Wahab**, M. Nawi, S.A. Hamid, R. Yusuf, N.A. Rahman, R. Othman, S. Othman

11:15 COMP 19. Computational study of 3-aryl-quinoxaline-2-carbonitrile 1,4-di-N-oxidide derivatives with anti-tumor properties. **E.M. Miller**, A. Nenninger, M.N. Mruzik, K.A. Brillos-Monia, P.W. Crawford, C. Ragain

Section D
New Orleans Marriott Convention Center
River Bend 2

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Data Mining & Frameworks for Chemical Discovery

Cosponsored by CINF and PHYS
D. Koes, E. Pyzer-Knapp, *Organizers, Presiding*

8:30 Introductory Remarks.

8:45 COMP 20. Pathway analysis and mode-of-action prediction based on computational modeling of high-throughput toxicogenomics. S. Haider, **K. Mansouri**, M.B. Black, P.D. McMullen

9:10 COMP 21. Automation approaches of large-scale systematic literature reviews to support performance-based validation of high throughput assays and biological pathway elucidation. **K. Markey**, A. Frame, C. Strope, S.R. Matten

9:35 COMP 22. Application of machine learning and computer vision techniques in information extraction and property predictions. **Y. Han**

10:00 COMP 23. "Lost in translation": Treating organic chemistry as a natural language. T. Gaudin, P. Schwaller, D. Lanyi, C. Bekas, **T. Laino**

10:25 Intermission.

10:40 COMP 24. Capturing and applying knowledge to guide compound optimisation. **M.D. Segall**, E. Champness, P. Hunt, T. Mansley

11:05 COMP 25. LiveDesign as a machine-learning platform for collaborative drug discovery. E. Davis, **C. Murphy**

11:30 COMP 26. Cognitive computing and machine learning for chemical & materials discovery. **J.W. Pitera**, D. Zubarev, C. Dai, S. Swaminathan

11:55 COMP 27. Development of a machine learning toolkit for drug discovery. **V. Tkachenko**, A. Korotcov, B. Sattarov, A. Mitrofanov, R. Zakharov

Section E
New Orleans Marriott Convention Center
Blaine Kern F

Large-Scale Applied Molecular Modeling
Cosponsored by CINF and MEDI
R. Alvarez, E. Metwally, *Organizers*
J.C. Alvarez, J. Duca, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COMP 28. Molecular simulation and machine learning for the design of finely tuned drugs. **R.O. Dror**

9:05 COMP 29. *In silico* prediction of diffusion interaction parameter (kD), a key determinant of antibody solution behaviors. **D. Tomar**

9:35 COMP 30. Protein mutagenesis and property optimization with MOE. **E. Metwally**

10:05 Intermission.

10:30 COMP 31. Using large-scale electronic structure modeling to understand unexpected interactions in the structurally characterized proteome. **H. Qi**, H.J. Kulik

11:00 COMP 32. Predicting allosteric back pocket tractability among protein kinases. **K.K. Brown**

Adventures in Density Functional Theory

Fundamental Properties of the Exact Density Functional

Sponsored by PHYS, Cosponsored by COMP‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Drug Discovery: Cheminformatic Approaches
Sponsored by CINF, Cosponsored by COMP

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL and PHYS

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Sponsored by PHYS, Cosponsored by

‡*Cooperative Cosponsorship*

COMP‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

SUNDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
New Levee

Molecular Mechanics

Sampling & Kinetics

M. Feig, *Organizer*
M. Niesen, *Presiding*

1:30 COMP 33. Tinker-HP: A massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced polarizable force fields. **J.A. Piquemal**

2:00 COMP 34. Microscopic derivation of particle-based coarse-grained dynamics: Exact expressions for dissipative interactions. **S. Izvekov**

2:30 COMP 35. Convergence of (multi-scale) free energy simulations. **G. Koenig**, D.M. York

3:00 Intermission.

3:15 COMP 36. Simulation study of long-timescale protein dynamics. **K. Corbett**, D. Wu, L. Zheng, W. Yang

3:45 COMP 37. Efficient phase space exploration by employing a local roundtrip-time optimisation for replica-exchange simulations. **D. Sidler**, M. Cristofol Clough, S. Riniker

4:15 COMP 38. Kinetic folding and binding networks from REMD trajectories. B. Narayan, C. Herbert, S. McCartan, B. Tywoniuk, Y. Yuan, A. Kells, E. Rosta, **N. Buchete**

4:45 COMP 39. Dimerization interfaces of the GPCR TGR5 revealed by integrative modeling. **C. Gertzen**, L. Waeschenbach, H. Gohlke

Section B
New Orleans Marriott Convention Center
Mississippi Queen

Computational Studies of Water

Phenomena

D.J. Sindhikara, *Organizer*
K.D. Ranasinghe, *Presiding*

1:30 COMP 40. Benchmark structures, energetics and harmonic vibrational frequencies of solvated halide and alkali metal ions. **G.S. Tschumper**

2:00 COMP 41. Connections between the anomalous volumetric properties of alcohols in aqueous solution and the volume of hydrophobic association. **H. Ashbaugh**

2:30 COMP 42. Nucleation tracking in aqueous environments. C. Williamson, **C.J. Fennell**

3:00 Intermission.

3:15 COMP 43. Coexistence of multilayered phases of confined water: The importance of flexible confining surfaces. **L.A. Ruiz Pestana**, L. Felberg, T.L. Head-Gordon

3:35 COMP 44. ReaxFF molecular dynamics simulations of electrolyte diffusion and polymer hydrolysis in ambient and supercritical water. **N. Dasgupta**, Y. Shin, A.C. Van Duin

3:55 COMP 45. Membrane desalination through silicon-passivated nanoporous graphene: A polarizable study. **Y. Qiu**, L. Wang

Section C
New Orleans Marriott Convention Center
Julia

Undergraduate Research & COMP Career Roundtable

M.C. Nagan, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 COMP 46. Introduction to molecular dynamics simulations. **J. Shen**

2:25 COMP 47. Introduction to quantum chemistry and QM simulations. **G.A. Cisneros**

3:15 Discussion.

4:05 Intermission.

4:20 Panel Discussion.

5:10 Concluding Remarks.

Section D
New Orleans Marriott Convention Center
River Bend 2

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Artificial Intelligent Searching of Chemical Space

Cosponsored by CINF and PHYS
D. Koes, E. Pyzer-Knapp, *Organizers, Presiding*

1:30 COMP 48. Molecular graph encoding convolutional neural networks for automatic chemical feature extraction. Y. Xu, **J. Pei**, L. Lai

1:55 COMP 49. Can androids dream of electric molecules? Generative models for chemistry and molecular properties. **A. Aspuru-Guzik**

2:20 COMP 50. Active search for computer-aided drug design. **J.D. Hirst**, S. Oatley, D. Oglic, T. Gaertner

2:45 COMP 51. Withdrawn

3:10 Intermission.

3:25 COMP 52. Coupling generative models to virtual screening: Application to organic redox flow batteries. **D.P. Tabor**, C. Outeiral, B. Sanchez-Lengeling, A. Aspuru-Guzik

3:50 COMP 53. Using machine learning to seed starting populations for evolutionary algorithm searches of organic structures. N. Kellas, **M. Groves**

4:15 COMP 54. Active learning in chemical space for the automatic improvement of the ANI deep learned potential with an application to reaction profiles. J.S. Smith, K.D. Ranasinghe, C. Devereux, O. Isayev, **A.E. Roitberg**

4:40 Panel Discussion.

Section E
New Orleans Marriott Convention Center
Blaine Kern F

Large-Scale Applied Molecular Modeling
Cosponsored by CINF and MEDI
R. Alvarez, J. Duca, *Organizers*
J.C. Alvarez, E. Metwally, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 COMP 55. Organic crystal structure prediction for industrial applications by a convergence-controlled blend of DFT-D with tailor-made force fields. **M.A. Neumann**

2:05 COMP 56. Molecular crystal structure prediction from large-scale first-principles calculations. **J. Hoja**, H. Ko, M.A. Neumann, R. Car, R.A. Distasio, A. Tkatchenko

2:35 COMP 57. Leveraging a large scale HPC environment for computational studies in catalyst design. **E.C. Sherer**

3:05 Intermission.

3:30 COMP 58. Studying nanoparticle-membrane interactions using MD simulations. **Z. Cournia**

4:00 COMP 59. Nonlinear modeling of organic compounds structures, simulation, and optimization of tandem mass spectrometer (MS) data. **F. Ochieng**, B.A. Logue, P. Hinker

4:30 COMP 60. Understanding passive membrane permeation with microsecond molecular dynamics. **C. Dickson**, V. Hornak, R.A. Pearlstein, J. Duca

Adventures in Density Functional Theory
Sponsored by PHYS, Cosponsored by COMP‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Carbon Dioxide Conversion & Artificial Photosynthesis
Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL‡ and PHYS

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Sponsored by PHYS, Cosponsored by COMP‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY MORNING

Section A
New Orleans Marriott Convention Center
New Levee

Computational Catalyst Design for Energy Conversion & Storage

Advances in Theory, Computational Models & Approaches

Cosponsored by CATL and CINF
C.M. Aikens, *Organizer*
C. Liu, *Organizer, Presiding*

8:00 COMP 61. Design of metal-organic framework catalysts beyond the active site. D. Gomez Gualdron, C.L. Whitford, P. Deria, P.C. Stair, R.B. Getman, J.T. Hupp, O.K. Farha, **R. Snurr**

8:40 COMP 62. Quantum mechanical description of excited-state catalysis on metals for nanoplasmonics. **J. Martirez**, E.A. Carter

9:10 COMP 63. Modeling catalytic reactions with multireference quantum chemical methods. **L. Gagliardi**

9:50 Intermission.

10:10 COMP 64. Theoretical design of molecular electrocatalysts with proton relays for energy conversion processes. **S. Hammes-Schiffer**

10:50 COMP 65. Predictive description of photo-induced electron transfer or transport through molecular-resolved interfaces. **B.D. Dunietz**

11:30 COMP 66. Design principles of materials for transformation and storage of energy. **J. Mendoza-Cortes**

Section B
New Orleans Marriott Convention Center
River Bend 2

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Cosponsored by CINF, MEDI and PHYS
Financially supported by Gaussian Inc. and OpenEye

G.A. Cisneros, *Organizer*
P. Tao, *Organizer, Presiding*
R. Swett, *Presiding*

8:30 Introductory Remarks.

8:40 COMP 67. Proton-coupled electron

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transfer in soybean lipoxygenase: Hydrogen tunneling, electrostatics, and conformational motions. **S. Hammes-Schiffer**

9:10 COMP 68. Insights on ALKB family native and cancer variant enzymes. **G.A. Cisneros**

9:40 COMP 69. Importance of electrostatic interactions in natural enzymes: What can we learn for enzyme design? T.A. Coulther, L. Ngu, P.J. Beuning, **M.J. Ondrechen**

10:10 Intermission.

10:25 COMP 70. Capturing and designing for electrostatic preorganization in enzymes. **A. Alexandrova**

10:55 COMP 71. Modeling the absorption spectrum of the chromophores of photoactive yellow protein (PYP) and green fluorescent protein (GFP) in water: Ensemble sampling, vibronic transitions, and nuclear quantum effects. **C. Isborn**, T. Zuehlsdorff

11:25 COMP 72. Comparison of catalytic mechanisms of multiple β-lactamases: Seeking chemical driving force behind antibiotic resistance. **P. Tao**, L. Shen

Section C
New Orleans Marriott Convention Center
Julia

Drug Design

QSAR & Docking

Cosponsored by CINF
M.R. Landon, Y. Tseng, *Organizers*
D. Ghoreishi, *Presiding*

8:30 COMP 73. MD-QSAR modeling of dynamic kinase-inhibitor interactions using machine learning and molecular dynamics trajectories. **D. Fourches**

9:00 COMP 74. Hydrophobic similarity between molecules: Application to three-dimensional molecular overlays with PharmScreen. J. Vazquez, A. Deplano, A. Herrero, E. Gibert, T. Ginex, O. Rabal, J. Oyarzabal, E. Herrero, **F. Luque**

9:30 COMP 75. ProBiSdock: Flexible docking using existing knowledge from the Protein Data Bank. **J. Konc**, D. Janezic

10:00 Intermission.

10:15 COMP 76. 'Middle-way' flexible docking: Combining mixed-resolution and non-equilibrium candidate Monte Carlo for improved pose prediction in estrogen receptor β. **J.M. Spiriti**, D.M. Zuckerman

10:45 COMP 77. Identifying drug binding sites on proteins from surface conservation and fragment docking. A.R. Vidad, S. Macaspac, **H. Ng**

11:15 COMP 78. Allosteric inhibition of the Zika virus NS3 helicase. **B. Raubenolt**, K. Wong, S. Rick

Section D
New Orleans Marriott Convention Center
Blaine Kern D

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Applied Machine Learning: Molecular Dynamics, Materials & Virtual Screening

Cosponsored by CINF and PHYS
D. Koes, E. Pyzer-Knapp, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COMP 79. Simultaneous learning and exploring potential energy surfaces. **A. Shapeev**, E.V. Podryabinkin, K. Gubaev, I.S. Novikov

9:00 COMP 80. Unsupervised clustering of molecules using minimum variance yields interpretable dynamical and structural groups. **B.E. Husic**, V.S. Pande

9:25 COMP 81. Using machine learning to automate calculations of conformational kinetics in molecular simulations. **G. Grazioli**, I. Andricioaei, C.T. Butts

9:50 Intermission.

10:05 COMP 82. Systematically identifying the best chemical representation for machine learning with applications in crystal structure prediction. **D. McDonagh**, C. Skylaris, G.M. Day

10:30 COMP 83. Prediction of scintillator light yield from composition using machine learning methods. **J. Garnett**, A. Burger

10:55 COMP 84. Data set expansion in consensus scoring for protein-ligand docking. S.S. Ericksen, F.M. Hoffmann, **S.A. Wildman**

Section E
New Orleans Marriott Convention Center
Blaine Kern F

Large-Scale Applied Molecular Modeling
Cosponsored by CINF and MEDI
J.C. Alvarez, R. Alvarez, *Organizers*
J. Duca, E. Metwally, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 COMP 85. Molecular modeling in the cloud: From billions to hundreds to one. **G.L. Warren**, A.G. Skillman, C.I. Bayly, T.A. Darden, A. Nicholls

9:05 COMP 86. Characterization of long-range interaction networks in proteins using key network principles. **Z. Haratipour**, H. Aldabagh, Y. Li, L.H. Greene

9:35 COMP 87. Leveraging cloud computing for large-scale QM calculations: Application to virtual screening and structure-based design. **B.K. Rai**, V. Sresht, Q. Yang, R. Unwalla, M. Tu, A. Mathiowetz, G.A. Bakken

10:05 Intermission.

10:30 COMP 88. Using MELD in flexible protein-protein docking. **E. Brini**, K. Dill

11:00 COMP 89. Macro-pKa calculations for complex tautomeric equilibria. **A. Bochevarov**, M.A. Watson, H.S. Yu

Adventures in Density Functional Theory

Conceptual Aspects

Sponsored by PHYS, Cosponsored by COMP‡

Carbon Dioxide Conversion & Artificial Photosynthesis

Theoretical Studies, Policy & Catalytic Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Sponsored by PHYS, Cosponsored by COMP‡

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL and PHYS

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
New Levee

Computational Catalyst Design for Energy Conversion & Storage

Development of Electro- & Photocatalysts

Cosponsored by CATL and CINF
C.M. Aikens, *Organizer*
C. Liu, *Organizer, Presiding*

1:30 COMP 90. Computational studies of reaction pathways for electrocatalytic CO_2 reduction to hydrocarbons on Cu-based catalysts. A.J. Garza, A.T. Bell, **M.P. Head-Gordon**

2:10 COMP 91. Characterization of NiFe oxyhydroxide electrocatalysts by integrated electronic structure calculations and spectroelectrochemistry. **G.A. Galli**

2:50 COMP 92. Computational design of non-precious transition metal/nitrogen doped carbon catalysts as fuel cell electrocatalysts. **G. Wang**

3:30 Intermission.

3:50 COMP 93. Theoretical investigations for CO2 reduction. **K. Chan**

4:30 COMP 94. Water oxidation in photosystem II characterized by a combined computational and experimental study of $^{16}O/^{18}O$ and H/D kinetic isotope effects. K.R. Yang, S. Khan, G.W. Brudvig, **V.S. Batista**

5:10 COMP 95. Orbitalwise coordination numbers as new descriptors for oxygen reduction catalyst design. **S. Wang**, H. Xin

Section B
New Orleans Marriott Convention Center
River Bend 2

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Cosponsored by CINF, MEDI and PHYS
Financially supported by Gaussian Inc. and OpenEye

P. Tao, *Organizer*
G.A. Cisneros, *Organizer, Presiding*
Q. Cui, *Presiding*

1:30 COMP 96. Hierarchical energy landscapes dictate protein functional motions. **W. Yang**

2:00 COMP 97. Free energy reservoirs: Short disordered protein regions. J. Drake, **B.M. Pettitt**

2:30 COMP 98. New approaches for overcoming ensemble mismatches in QM/MM free energy simulations. P. Hudson, F. Kearns, S. Boresch, **H.L. Woodcock**

3:00 Intermission.

3:15 COMP 99. Multiscale approaches combining quantum chemistry and polarizable classical models: Applications to biological systems. **B. Mennucci**

3:45 COMP 100. Hybrid QM/MM molecular dynamics with AMOEBA polarizable embedding for enzyme studies. **J.A. Piquemal**

4:15 COMP 101. Uncovering the quantum mechanical origins of enzymatic catalysis with systematic QM/MM methods and accelerated, large-scale electronic structure. **H.J. Kulik**

Section C
New Orleans Marriott Convention Center
Julia

Drug Design

Molecular Property

Cosponsored by CINF
M.R. Landon, Y. Tseng, *Organizers*
A. Aderibigbe, *Presiding*

1:30 COMP 102. Halide bonds in drug discovery: Really that important? **C. Detering**, M. Gastreich

2:00 COMP 103. Quantum chemical pKa prediction for conformationally flexible drug molecules. **A. Bochevarov**, D.M. Philipp, T.B. Steinbrecher, M.A. Watson, H.S. Yu

2:30 COMP 104. Critical assessment of the performance of automated pharmacophore hypotheses derived from series of ligands and protein-ligand complexes. E. Mack, **M.R. Landon**, S.L. Dixon, M.P. Repasky

3:00 Intermission.

3:15 COMP 105. High-throughput prediction of fraction absorbed and bioavailability *in silico*. **R. Fraczkiewicz**, P.R. Daga, R.D. Clark

3:45 COMP 106. Unique hydrophobic binding sites dominate substrate specificity: A significant discovery for developing phospholipase inhibitors. **V. Mouchlis**, J. McCammon, E.A. Dennis

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4:15 COMP 107. Intramolecular hydrogen bond impact on permeability via matched molecular pair analysis. **F. Ruggiu**, J.E. Prescott-Roy, J.M. Jansen

Section D
New Orleans Marriott Convention Center
Blaine Kern D

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Deep Learning for Deep Chemical Understanding

Cosponsored by CINF and PHYS
D. Koes, E. Pyzer-Knapp, *Organizers, Presiding*

1:30 COMP 108. Deep learning for molecular docking. **D. Koes**

1:55 COMP 109. ChemNet: A transferable and generalizable deep neural network for small-molecule property prediction. C. Siegel, A. Vishnu, N. Hodas, **G. Goh**

2:20 COMP 110. Applications of convolutional neural networks for computational chemistry. **V. Tkachenko**, B. Sattarov, A. Korotcov, A. Mitrofanov, R. Zakharov

2:45 COMP 111. DLScore: New deep learning based scoring function for reliable protein-ligand scoring. **S. Sirimulla**, G. Muela, O. Fuentes

3:10 Intermission.

3:25 COMP 112. Molecular machine learning with DeepChem. **B. Ramsundar**

3:50 COMP 113. Machine learning for inorganic molecular design: Descriptors and similarity in transition metal chemical space. **J. Janet**, H.J. Kulik

4:15 COMP 114. AIMNet: Accurate universal neural network potential for atomic energies, charges and polarizabilities. **R. Zubatyuk**, J.R. Leszczynski, O. Isayev

4:40 COMP 115. Distilling chemical knowledge from neural network potentials. **O. Isayev**

5:05 Panel Discussion.

Section E
New Orleans Marriott Convention Center
Blaine Kern F

Large-Scale Applied Molecular Modeling
Cosponsored by CINF and MEDI
R. Alvarez, *Organizer*
J.C. Alvarez, J. Duca, E. Metwally, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 COMP 116. Molecular dynamics with machine learning potentials. From gas phase to solution chemistry, at low cost and high accuracy. **A.E. Roitberg**

2:05 COMP 117. Multilayer divide-expand-consolidate methods applied to the study of gas adsorption in Mg-based metal-organic frameworks (MOF-74). **A.L. Barnes**, D. Bykov, D. Liakh, T. Straatsma

2:35 COMP 118. How GPUs are driving large-scale molecule modeling and machine learning (ML). **M.E. Berger**

3:05 Intermission.

3:35 COMP 119. Interpretation of structure-activity relationship in congeneric series using the linear response approximation and free energy decomposition. **N.V. Plotnikov**

4:05 COMP 120. Biosignature-based drug design: A new drug design paradigm. **J. Wegner**

Adventures in Density Functional Theory

Weak Interactions

Sponsored by PHYS, Cosponsored by COMP‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Carbon Dioxide Conversion & Artificial Photosynthesis
Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Machine Learning for Catalysis Research
Sponsored by CATL, Cosponsored by CINF and COMP

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Sponsored by PHYS, Cosponsored by COMP‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
H.L. Woodcock, *Organizer*

8:00–10:00

172, 174-176, 179, 184, 190, 192, 195, 203, 205, 212, 217-219, 227, 231, 245, 249, 256-257, 264, 272, 276, 281, 285, 291, 295, 298, 302, 307, 311, 316, 320-324, 327, 329.
See subsequent listings.

TUESDAY MORNING

Section A
New Orleans Marriott Convention Center
Blaine Kern F

Computational Catalyst Design for Energy Conversion & Storage

Development of Homogeneous & Heterogeneous Catalysts

Cosponsored by CATL and CINF
C.M. Aikens, *Organizer*
C. Liu, *Organizer, Presiding*

8:00 COMP 121. Adventures in redox non-innocent ligands & earth-abundant transition metal catalysts. **T.R. Cundari**

8:40 COMP 122. Understand the role of solvent effects in the thermal and electrochemical hydrogenation of carbonyls. **R. Rousseau**, V. Glezakou, M. Lee, D.C. Cantu, S. Akhade, M. Nguyen

9:20 COMP 123. Molecular simulations for calculating the free energies of adsorption and reaction in aqueous phase heterogeneous catalysis. X. Zhang, **R.B. Getman**

10:00 Intermission.

10:20 COMP 124. Tuning activity and selectivity of Cu-based catalysts toward CO_2 reduction. S. Kattel, J.G. Chen, J. Rodriguez, **P. Liu**

11:00 COMP 125. S_E2 reaction for non-carbon system: Ammonia borane dehydrogenation by homogeneous catalysts. **S. Pai**, S. Han

Section B
New Orleans Marriott Convention Center
River Bend 2

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Cosponsored by CINF, MEDI and PHYS
Financially supported by Gaussian Inc. and OpenEye

G.A. Cisneros, P. Tao, *Organizers*
C. Isborn, J.A. Piquemal, *Presiding*

8:30 COMP 126. Allostery along the ATP hydrolysis cycle of dengue viral NS3 helicase. **M. McCullagh**

9:00 COMP 127. Flexible-body interaction of farnesylated HVR with calmodulin enables K-Ras4B membrane extraction. **R. Nussinov**, H. Jang

9:30 COMP 128. Application of parallel continuous simulated tempering (PCST) to cryo-EM structural refinement at near-atomic resolution. **J. Ma**

10:00 Intermission.

10:15 COMP 129. Exploring the flexibility of extremophile enzymes by molecular dynamics simulations. **T. Ichiye**

10:45 COMP 130. Chemical and conformational transformations in enzymes. **Q. Cui**

11:15 COMP 131. Effects of a single point mutation and mismatched base on DNA polymerase III holoenzyme proofreading. **A. Walker**, H. Gahlon, D. Rueda, G.A. Cisneros

Section C
New Orleans Marriott Convention Center
Julia

Molecular Mechanics: Computational Studies of Transmembrane Proteins

M. Feig, J. Shen, *Organizers*
J.V. Vermaas, *Presiding*

8:30 COMP 132. Complexity of gating dynamics in biological nanopores: Case of voltage-dependent anion channel (VDAC1). V. Ngo, T. Rostovtseva, S. Bezrukov, **S. Noskov**

9:00 COMP 133. Influence of pore-lining residues on ion transport through channelrhodopsins. **M. VanGordon**, S.W. Rick, C. Rempe, M. Chaudhari, S.L. Rempe

9:30 COMP 134. Refining amino acid hydrophobicity for dynamics simulation of membrane proteins. **R.D. Hills**

10:00 COMP 135. Cholesterol condensation using ELBA coarse graining. **S. Wheeler**, J. Essex

10:20 Intermission.

10:35 COMP 136. Modeling of the pH-dependent process in the integral membrane influenza A proton channel (AM2) using constant pH molecular dynamics simulations. **H. Torabifard**, A. Panahi, C.L. Brooks

11:05 COMP 137. Detailed mechanism of proton-driven sodium transport across the membrane. **O. Beckstein**

11:35 COMP 138. Signaling pathways in transmembrane receptors deduced from network rigidity. **C. Pfleger**, H. Gohlke

11:55 COMP 139. Membrane allostery and hydrophobic binding sites control substrate specificity of lipolytic enzymes. **V. Mouchlis**, E.A. Dennis, J. McCammon

Section D
New Orleans Marriott Convention Center
Blaine Kern D

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Jürgen Bajorath
Cosponsored by CINF and MEDI
J. Bajorath, *Organizer*
V. Shanmugasundaram, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COMP 140. Exploring latent information in drug-target databases and networks. **G.M. Maggiora**, V. Gokhale

9:05 COMP 141. Development of a knowledge-generating platform driven by big data in drug discovery through production processes. **K. Funatsu**

9:35 COMP 142. Cleansing drug discovery data for data science predictive modeling. **T.R. Stouch**

10:05 Intermission.

10:20 COMP 143. D-Tools: Open resources for chemical space and global diversity analysis of compound databases. **J.L. Medina-Franco**, M. González-

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Medina

10:50 COMP 144. From activity cliffs to promiscuity cliffs. **D. Dimova**

11:20 COMP 145. Molecular design and informatics for all. **C. Kreatsoulas**

Adventures in Density Functional Theory

Strong Correlation

Sponsored by PHYS, Cosponsored by COMP‡

Dreyfus Prize Symposium

Theory & Computation

Sponsored by MPPG, Cosponsored by COMP‡, PHYS‡ and PRES

Carbon Dioxide Conversion & Artificial Photosynthesis

Photocatalytic Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Cheminformatics Resources & Software Tools Supporting Environmental Chemistry
Sponsored by CINF, Cosponsored by COMP and ENVR

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Sponsored by CATL, Cosponsored by COMP and ENFL

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Sponsored by PHYS, Cosponsored by COMP‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
Blaine Kern F

Computational Catalyst Design for Energy Conversion & Storage

Development of Homogeneous & Heterogeneous Catalysts

Cosponsored by CATL and CINF
C.M. Aikens, *Organizer*
C. Liu, *Organizer, Presiding*

1:30 COMP 146. Tuning 2D materials MoS_2 and h-BN for hydrogenation reactions. D. Le, T.B. Rawal, T. Jiang, **T.S. Rahman**

2:10 COMP 147. Plasma-assisted catalysis: Understanding the effect of excitations on rates and optimal catalysts. P. Mehta, P. Barboun, F. Herrera, J. Kim, D. Go, J.C. Hicks, **W.F. Schneider**

2:50 COMP 148. Designing functionalized metal organic frameworks for carbon dioxide capture and hydrogenation. **K. Johnson**, J. Ye, L. Li

3:30 Intermission.

3:50 COMP 149. Revealing biomass catalytic fast pyrolysis upgrading: from diffusion to reaction classes. L. Bu, B. Knott, M.R. Nimlos, D. Robichaud, **S. Kim**

4:30 COMP 150. Atomistic scale modeling for catalytic vapor phase upgrading of bio oil components. **R. Surendran Assary**, L.A. Curtiss, D. Pahls, B. Narayanan

Section B
New Orleans Marriott Convention Center
River Bend 2

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Cosponsored by CINF, MEDI and PHYS
Financially supported by Gaussian Inc. and OpenEye

G.A. Cisneros, P. Tao, *Organizers*
M. McCullagh, *Presiding*

1:30 COMP 151. Profiling cathepsin D and BACE2: Flap dynamics and interaction with a BACE1 inhibitor. **J. Shen**, J. Henderson, C. Tsai

2:00 COMP 152. Decomposing cooperativity into stabilizing and destabilizing effects upon site directed mutations. **D.J. Jacobs**

2:30 COMP 153. Multiscale modeling and network-based systems biology analysis of protein kinase regulation by the Hsp90-Cdc37 chaperone system: Towards discovery of synergistic allosteric modulators targeting Hsp90-kinase interactions and evading drug resistance. **G. Verkhivker**

3:00 Intermission.

3:15 COMP 154. Application of biomolecular simulation to industrial drug design. **R. Swett**

3:45 COMP 155. Structural modeling and thermodynamic characterization of a D-Pro-Pro-Glu-NH2 catalytic peptide / reactant emulsion: A comparison to modern enzymes. L. Wang, **B.N. Dominy**

4:15 COMP 156. Allosteric effects in a catalytically impaired variant of cyclophilin A are unrelated to millisecond time scale motions. **J. Michel**, P. Wapeesittipan, A. Mey, M. Walkinshaw

4:45 Concluding Remarks.

Section C
New Orleans Marriott Convention Center
Julia

Quantum Mechanics

A.E. DePrince, *Organizer*
H.P. Hratchian, *Presiding*

1:30 COMP 157. NOF-MP2: Global method for electron correlation. **M. Piris**

2:00 COMP 158. Weak and strong correlation contributions to the Coulomb Hole. **E. Matito**

2:30 COMP 159. Hybrid cumulant-density functional for chemistry. **J.W. Hollett**, N. Pegoretti

3:00 COMP 160. Dynamical correlation models for variational two-electron reduced-density-matrix driven complete active space self-consistent field methods. **A.E. DePrince**

3:30 Intermission.

3:45 COMP 161. Large-scale wavefunctions for electronics and biology. **T.R. Clark**

4:15 COMP 162. Modeling ground and excited-state electron dynamics in large chemical systems using real-time propagation of semiempirical effective Hamiltonian. **S. Ghosh**, J.C. Asher, L. Gagliardi, C.J. Cramer, N. Govind

4:35 COMP 163. Capturing plasmon/polariton dynamics of molecular dye monolayers on metallic core-shell nanoparticles using classical electrodynamics with quantum embedding. **H.T. Smith**, T.E. Karam, L.H. Haber, K. Lopata

4:55 COMP 164. Wavelength and intensity dependence of recollision-enhanced multielectron effects in high-harmonic generation. **P. Abanador**, F. Mauger, K. Lopata, M. Gaarde, K. Schafer

Section D
New Orleans Marriott Convention Center
Blaine Kern D

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Jürgen Bajorath
Cosponsored by CINF and MEDI
J. Bajorath, *Organizer*
V. Shanmugasundaram, *Organizer, Presiding*

1:30 COMP 165. Forward-looking strategy on how can chemistry and informatics enable biology. **M. Glick**

2:00 COMP 166. Data-driven design: From matched pairs to multiobjective modeling. **S. Posy**, M. Pokross

2:30 COMP 167. All problems solved? On the quest for algorithms in cheminformatics and structure-based design. **M. Rarey**

3:00 Intermission.

3:15 COMP 168. Show me; don't tell me: Data visualization in computational chemistry. **G. McGaughey**

3:45 COMP 169. More numerous than the stars in the sky: Breadth of chemical claims in pharmaceutical patents. **P. Walters**, M. Murcko

4:15 COMP 170. Protein degradation: Hijacking the ubiquitin-proteasome system. **V. Shanmugasundaram**

4:45 COMP 171. Award Address
(ACS Award for Computers in Chemical and Pharmaceutical Research Sponsored by the ACS Division of Computers in Chemistry). Revisiting the scaffold concept: An oldie, but goodie. **J. Bajorath**

Dreyfus Prize Symposium

Theory & Computation

Sponsored by MPPG, Cosponsored by COMP‡, PHYS‡ and PRES

Cheminformatics Resources & Software Tools Supporting Environmental Chemistry
Sponsored by CINF, Cosponsored by COMP and ENVR

Carbon Dioxide Conversion & Artificial Photosynthesis

Electro-Photo Catalytical Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall E

Chemical Computing Group Graduate Student Travel Awards

K.N. Kirschner, C.L. Simmerling, *Organizers*

6:00–8:00

COMP 172. Pummerer-like rearrangement: Effects of solvent on a post-transition state bifurcation. **S.R. Hare**, D.J. Tantillo

COMP 173. Mixing oil and water: The thermodynamics and mechanism of water transferring into oil. **J.J. Karnes**, I. Benjamin

COMP 174. Forces on nascent polypeptides during membrane insertion and translocation via the Sec translocon. **M. Niesen**, T.F. Miller

COMP 175. Unfolding pathways of hen egg white lysozyme in ethanol; insights from IMS-MS and molecular dynamics. **A. Walker**, D.W. Woodall, E. Inutan, N. Baddam, P. Stemmer, S. Trimpin, G.A. Cisneros

COMP 176. Enabling and accelerating Hessian calculations with numerical nuclear second derivatives on computing grid. **T. Yang**, J.F. Berry

Section A
Ernest N. Morial Convention Center
Hall E

COMP Poster Session

H.L. Woodcock, *Organizer*

6:00–8:00

COMP 177. Docking study of DDT and analogues in the androgen and estrogen receptor BF-3 surface binding site. **A.R. Cruz**, M.D. Rosales, F. Dean, E. Kotsikorou

COMP 178. Mapping ligand binding landscapes with WExplore. **A. Dickson**

COMP 179. Functional assignment of structural genomics proteins through computed chemical properties, graph representation of active sites, and

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biochemical validation. **C.L. Mills**, R. Garg, J. Lee, R. Parasuram, L. Tian, A. Suciu, G. Cooperman, P.J. Beuning, M.J. Ondrechen

COMP 180. Design of novel inhibitors for the aldehyde dehydrogenases. **C. Magee**, L.W. Peterson, M.L. Cafiero

COMP 181. Modeling molecular flux in nano-particle assisted drug deliver. **C. Leehy**, S. Poh, E. Sherer

COMP 182. Molecular dynamics simulation of biased agonists at the dopamine D2 receptor suggests the mechanism of receptor functional selectivity. **C. Wu**

COMP 183. Simulating the binding pathways of sialic acid and oseltamivir to h274y neuraminidase with molecular dynamics simulations. **D. Dacres**, E. Lewis, R. Wenner, A.W. Van Wynsberghe

COMP 184. @CompChemBot: Exploring the textual landscape of computational chemistry. **E.X. Esposito**

COMP 185. Analysis of MM/GBSA free energy calculations to investigate the binding pathways of neuraminidase. **E. Lewis**, P. Marris, L.M. Krause, A.W. Van Wynsberghe

COMP 186. Weighted averaging scheme for pKa prediction based on density functional theory. **H. Yu**, M.A. Watson, A. Bochevarov

COMP 187. Efficient approach for finding fragment-binding poses. **H. Sato**, Y. Tanida, A. Matsuura

COMP 188. ProBiS tools on GPU accelerators. **J. Konc**

COMP 189. Exploration of the binding kinetics of Zanamivir to WT neuraminidase via computational analysis of molecular dynamics simulations. **K.L. Nash**, R. Wenner, A.W. Van Wynsberghe

COMP 190. Extending an automated transition state search to locate low energy conformers of the transition state ensemble and application to the determination of intrinsic reactivity of covalent inhibitors. **L.D. Jacobson**, A. Bochevarov

COMP 191. Alternative network architectures for protein-ligand scoring. **L. Turner**, P. Mittal, M. Ragoza, D. Koes

COMP 192. Adding pharmacophores to shape and electrostatics–too much of a good thing? **M. Slater**, M.D. Mackey, T. Cheeseright, S. Tomasio

COMP 193. Computational analysis of non-nucleoside containing molecules as potential inhibitors of LpxC. **R. Roldan**, C. Dishuck, L.W. Peterson, M.L. Cafiero

COMP 194. Advancing drug discovery with free energy calculations. **R. Abel**, L. Wang, S. Bhat, S. Mondal, J. Knight, K. Konze, A. Clark

COMP 195. Phantom PAINS: Problems with the utility of alerts for Pan-Assay INterference CompoundS. **S. Capuzzi**

COMP 196. Predicting drug–drug interactions through drug structural similarities and interaction networks incorporating pharmacokinetics and pharmacodynamics knowledge. **T. Takeda**, M. Hao, T. Cheng, S.H. Bryant, Y. Wang

COMP 197. Novel drug design for Chagas disease via targeting *T. cruzi* tubulin: Pharmacophore studies to enhance the selectivity of naphthoquinone based inhibitors. C. Ogindo, O. Bakare, M. George, JR, C. Lee, W.M. Southerland, **Y. Fang**

COMP 198. Conformational flexibility in solution: Benchmarking conformer generators against a new ROESY NMR dataset. **F. Ruggiu**, M. Pillong, J.M. Jansen

COMP 199. Identifying unique HIV-1 entry inhibitor leads using virtual screening and docking techniques. **N. Gupta**, C.F. Abrams

COMP 200. Integrated screening for arginase inhibitors. **J.H. Audie**, T. Sullivan, B.J. Alper

COMP 201. Computational design of novel insulin degrading enzyme inhibitors. **T. Sullivan**, B.J. Alper, J.H. Audie

COMP 202. Drug designing for hormone therapy resistant breast and prostate cancers. P.K. Biswas, **R. Williams**

COMP 203. Predicting protein-protein binding sites and epitope mapping. **A. Ajamian**

COMP 204. Protocol for the analysis of vibrational circular dichroism spectra of small molecules using Gaussian and MOE. **A. Ajamian**

COMP 205. Catalysis in the Varkud satellite ribozyme. **A. Ganguly**, D.M. York

COMP 206. Computational study of magnesium ion coordination in the mechanism of HIVRT Polymerase. **A. Chang**, S. Kirmizialtin

COMP 207. Investigation of various computational methods for computing solvation energetics of phosphorus based extractants. **A.T. Ta**, B.D. Etz, G.A. Hegde, S. Vyas

COMP 208. Double-stranded protonated Poly(rA) RNA complex – computational studies. **A. Golius**, L. Gorb, M. Zarudnaya, A. Potyahaylo, J.R. Leszczynski

COMP 209. Molecular dynamics study of cyclopentane-modified peptide nucleic acids. **A. Manukyan**

COMP 210. Development of coarse-grained model for carboxylic acid. **A. Sharma**, G. Gyawali, S.W. Rick

COMP 211. Effect of mutations in osteogenesis imperfecta on structural stability of collagen. **A. Mekkat**, H. Yu, B. Brodsky, Y. Lin

COMP 212. Reaction path-force matching in collective variables: Determining *ab initio* QM/MM free energy profiles for solution-phase reactions. **B. Kim**, M. Nagaraju, Y. Zhou, P. Ojeda-May, S. Keeton, M. Hege, J. Pu

COMP 213. Multiple-time-step molecular dynamics in fragment-based calculations. **B. Westheimer**, M.S. Gordon

COMP 214. MMPBSA calculations of small RNA molecules containing 3′ overhangs. **C. Velez**, M.C. Nagan

COMP 215. Computational RNA enzymology: New tools to unravelling the catalytic mechanism of nucleolytic ribozymes. **C.S. Gaines**, D.M. York

COMP 216. Accelerating nudged elastic band method for finding minimum energy paths. **D. Ghoreishi**, D.S. Cerutti, A.E. Roitberg

COMP 217. Anisotropic reaction field correction for long-range electrostatic interactions in molecular dynamics simulations. **D. Sidler**, S. Frasch, M. Cristofol Clough, S. Riniker

COMP 218. Exploration of protein electrostatics through the interpretation of pH dependent NMR chemical shift perturbations. **E. Artikis**, C.L. Brooks

COMP 219. Using information to reduce the phase space of molecular dynamic simulations of biologically relevant problems. **E. Brini**, A. Perez, J.C. Robertson, C. Liu, R. Nassar, K. Dill

COMP 220. Interfacial ionic partitioning and its impact on small reverse micelles. **G. Prelvukaj**, **E. Tale**, A.K. Sharma

COMP 221. Using topology of molecular solvation for biomolecular structural refinement. **G.M. Giambasu**

COMP 222. Anion effects on oligomer formation of cytochrome *c* with MD simulation and 3D-RISM theory. **H. Motoki**, N. Yoshida, S. Hirota, M. Higashi

COMP 223. Functionally relevant intrinsic dynamics in prolyl-tRNA synthetase. **H. Hu**, S. Hati, **S. Bhattacharyay**

COMP 224. CgProt parameters for the simulation of ion-membrane interactions. **J. White**, K.A. Chalmers, R.D. Hills

COMP 225. Binary pressure-composition phase behavior of supercritical carbon dioxide + organic compounds from Monte Carlo molecular simulation. M. Huber, **J.M. Stubbs**

COMP 226. Visualizing convolutional neural network scoring of protein-ligand binding. **J. Hochuli**, **A. Helbling**, M. Ragoza, D. Koes

COMP 227. Understanding long-timescale ionization coupled dynamics of thioredoxin. **K. Corbett**, L. Zheng, D. Wu, W. Yang

COMP 228. Investigating the impact of metal binding modes on ribozyme catalysis through the use of GPU-accelerated simulations. **K. Kostenbader**, D.M. York

COMP 229. Investigating the interactions of the pilin ComP with DNA using molecular dynamics simulations. **K. Patel**, M. Fairfield, J.L. Baker

COMP 230. Investigating the effect of ionic liquids on drug transport in lipid bilayers. **K. Vogt**, A.J. Heyert, G.E. Lindberg, J.L. Baker

COMP 231. Movable type method: A fast, free energy method for scoring, docking, and conformational search. **L. Westerhoff**, Z. Zheng, K.M. Merz

COMP 232. Free energy calculations of membrane translocation: Finding, overcoming, and learning from convergence bottlenecks. **L. Maibaum**

COMP 233. Quantitative evaluation of site energies and their fluctuations of pigments in the light-harvesting complex with an efficient method for generating a potential energy surface. **M. Higashi**, S. Saito

COMP 234. MD and 3D-RISM approach to the ion transport of channel rhodopsin. **N. Yoshida**, C. Cheng, S. Hayashi

COMP 235. Improvised catalytic mechanism of *E. coli* glycinamide ribonucleotide transformylase: A computational study. **P. Gupta**, A.E. Roitberg

COMP 236. Novel computational methods to explore protein allostery: Rigid residue scan and machine-learning methods. **P. Tao**

COMP 237. Understanding allosteric regulation of human ribonucleotide reductase through computational studies. **P. Buteler**, A.E. Roitberg, M. Harris

COMP 238. Revealing substrate positioning dynamics in aliphatic halogenase SyrB2 through spectroscopically-guided simulation. **R. Mehmood**, H.J. Kulik, H. Qi

COMP 239. Molecular dynamics studies of *Vibrio cholerae* protein H-NOX. **R. Mukhopadhyay**

COMP 240. Computational investigation of cancer-related mutations on DNA polymerase β. **S. Maier**, P. Silvestrov, G. Cisneros

COMP 241. Dielectric balancing of molecules improves liquid-state and molecular transfer properties. **S. Paranahewage**, C. Gierhart, C. Fennell

COMP 242. Effect of the distributed partial wave expansion on the solvation free energy in the 3D-RISM theory. **S. Tanimoto**, N. Yoshida, H. Nakano

COMP 243. All-atom molecular dynamics of an ion-channel formed by viral protein U in lipid bilayers. **S. Wang**, I.R. Gould

COMP 244. Simulating nucleic acids in their crystal environment: A test for gauging accuracy of modern force fields. **S. Ekesan**, D.M. York

COMP 245. Molecular dynamics study of gearing and slippage motions in molecular spur gears. **S. Yang**, T. Liu, X. Jiang, P. Yu, M.J. Jellen, M.A. Garcia-Garibay, K.N. Houk

COMP 246. Computational study of alkene reduction in old yellow enzymes. **S. Lenka**, P. Buteler, R. Powell, J.D. Stewart, A.E. Roitberg

COMP 247. Membranes allosterically regulate substrate specificity of lipolytic enzymes. **V. Mouchlis**, J. McCammon, E.A. Dennis

COMP 248. Withdrawn

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COMP 249. High-performance multidimensional replica exchange molecular dynamics along pH, redox potential and temperature dimensions using AMBER. **V.D. Cruzeiro**, A.E. Roitberg

COMP 250. Characterizing the folding and misfolding of the *Aquifex Aeolicus* tmRNA frameshifting pseudoknot via massively parallel molecular dynamics simulations. **X. Martinez**, K. Nguyen, M. Bakhom, E.J. Sorin

COMP 251. Evolutionarily conserved and divergent residue-residue contact dynamics provide insights into the allosteric regulation of cyclophilins. P.J. Vu, **X. Yao**, M. Momin, D. Hamelberg

COMP 252. Computational studies of membrane interaction of hIAPP aggregates: Implication of different membrane-disruption mechanisms. **Y. Liu**, B. Ren, M. Zhang, Y. Zhang, F. Yang, J. Zheng

COMP 253. Alchemical free energy calculation via metadynamics. **Y. Tanida**, A. Matsuura

COMP 254. Withdrawn

COMP 255. Basis set convergence of harmonic vibrational frequencies for simple hydrogen bonded systems with atomic natural orbital basis sets. **A.O. Denette**, T.M. Sexton, G.S. Tschumper

COMP 256. Elucidation of CID fragment identities and properties for mass spectrometric studies of peptides. **A.S. McNeill**, C. Cui, S. Miller, M. Stover, C.J. Cassady, **D.A. Dixon**

COMP 257. Finding stable and metastable uranium oxides: Predicting UO_x crystal structures with genetic algorithms and DFT. **A. Shields**, A. Miskowiec, B. Anderson

COMP 258. Retention of conjugation in monomacrocyclic dendrimers with ether and amine bridges. **A.R. Smyly**, B. Nash, T.D. Selby, D.H. Magers, S.A. Smith

COMP 259. DFT study of the selectivity of mutated monoamine oxidase B (MAOB) for novel ligands. **A. Woody**, S.N. Jelinek, L.W. Peterson, M.L. Cafiero

COMP 260. Relative energies and conventional strain energies of the oxaphosphetanes and the oxadiphosphetanes. **B. Nash**, M. Westrope, D.H. Magers, S.A. Smith

COMP 261. Computational examination of the reaction channels of non-heme iron(IV)-oxo species. **B. Casale**, K.D. Vogiatzis

COMP 262. Solvation of isoelectronic atomic ions by noble gas atoms. **C.A. Rock**, G.S. Tschumper

COMP 263. Analysis of the relative energies of isomers of diphosphetane in terms of attractive versus repulsive forces. **C.R. Noel**, S.A. Smith, D.H. Magers

COMP 264. Determining molecular normal modes and geometry optimization using the deep learning method ANAKIN-ME. **C. Devereux**, J.S. Smith, O. Isayev, A.E. Roitberg

COMP 265. Characterization of azirine (C_2H_3N) and its isomers. **C. Dickerson**, P. Bera, T.J. Lee

COMP 266. New metrics for the reactivity and stability of antioxidant fullerenols found using the Born-Haber cycle. **D. Mulvey**, K. Lewis

COMP 267. Impact of molecular vibrations on exciton energy transfer in the phycoerythrin protein complex. **D. Kosenkov**

COMP 268. DFT study of the selectivity of DOPA-decarboxylase. **E. Harrison**, A.R. Ritter, M.L. Cafiero, L.W. Peterson

COMP 269. DFT analysis of water clusters, dopaminergic derivatives, and their desolvation energies. **E. Sanders**, M. Morris, L.W. Peterson, M.L. Cafiero

COMP 270. Toward QM/MM simulations using the Gaussian electrostatic model. **H. Gokcan**, E.G. Kratz, T.A. Darden, J.A. Piquemal, G. Cisneros

COMP 271. Applicability of effective fragment potential version 2–molecular dynamics (EFP2-MD) simulations for predicting excess properties of mixed solvents. N. Kuroki, **H. Mori**

COMP 272. Hybrid quantum-classical model of electrostatics in multiply charged quantum dots. **H. Liu**, D.R. Gamelin, X. Li

COMP 273. Enthalpies of formation of methyl derivatives of furan, pyrrole, oxazole, isoxazole, and imidazole by homodesmotic reactions. **J. Bethea**, C.D. Lewis, E.Q. Chong, S.A. Smith, D.H. Magers

COMP 274. Conventional strain energies of thiaziridine and the thiazetidines. **J.D. Gramm**, S.A. Smith, D.H. Magers

COMP 275. Predictions of brominated halocarbon bond dissociation energies via *ab initio* methods. **K.R. Jorgensen**

COMP 276. ANAKIN-ME: Using deep learning to develop a chemically accurate and universal potential for the prediction of organic reactions. **K.D. Ranasinghe**, J.S. Smith, O. Isayev, A.E. Roitberg

COMP 277. DFT analysis of the selectivity of phenylalanine hydroxylase. **M.C. Perchik**, R.M. Giampapa, L.W. Peterson, M.L. Cafiero

COMP 278. Engineering an automatic workflow for a DFT-based macro-pKa predictor including conformational and tautomeric effects. **M.A. Watson**, D.M. Philipp, H.S. Yu, A. Bochevarov

COMP 279. Photochemical properties of vitamin B_{12} derivatives: Implications from TD-DFT calculations. **M.J. Toda**, P. Lodowski, K. Ciura, M. Jaworska, P.M. Kozlowski

COMP 280. Many-body dispersion. **M. Alkan**, P. Xu, M.S. Gordon

COMP 281. New adventures in gas phase iron diatomic electronic spectroscopy. **N.J. Deyonker**, M.K. Bassett, Q. Cheng

COMP 282. Quantifying metal-nitrosyl coordination modes and oxidation states through X-ray emission spectroscopy and density functional theory. **P. Phu**, S. Kundu, S.E. Stieber, T.H. Warren

COMP 283. Effect of mutations on the binding of ligands in phenylalanine hydroxylase. **R.M. Giampapa**, L.W. Peterson, M.L. Cafiero

COMP 284. Evaluation of hybrid and pure DFT methods for the binding of novel ligands in the tyrosine hydroxylase enzyme. **R. Evans**, L.W. Peterson, M.L. Cafiero

COMP 285. Enhanced ionization of peptides using trivalent metals: Developing the basis for proteomics studies. **R.R. Persaud**, C. Rogers, E. Hartmann, S.N. Lambert, C.J. Cassady, **D.A. Dixon**

COMP 286. Energetics and vibrational signatures of nucleobase argyrophilic interactions. **S. Lee**, G.S. Tschumper

COMP 287. DFT study of the selectivity of monoamine oxidase B. **S.N. Jelinek**, A. Woody, L.W. Peterson, M.L. Cafiero

COMP 288. Noncovalent interactions between trimethylamine *N*-oxide (TMAO), urea, and water. **S. Travis**, J. Bethea, L. Boutwell, N. Hammer, S.A. Smith, D.H. Magers

COMP 289. Conventional strain energies of thiirane, thietane, borylthiirane, 2-borylthietane, and 3-borylthietane. **S.L. Nash**, M.M. Mohamed, S.A. Smith, D.H. Magers

COMP 290. Two-dimensional DFT potential energy surface scans for formamide and related derivatives: Studying the degree of nitrogen inversion during C-N bond rotation. M. Ma, **W.T. Grubbs**

COMP 291. Theoretical study on the selectivity of post-transition state bifurcation reactions. **X. Dong**, Z. Yang, K.N. Houk

COMP 292. Withdrawn

COMP 293. Conformational analysis of 1,2-dialkyl-2,3-epoxy cyclopentanol diastereomers. **Y.A. Abdo**, J.W. Weeks, J.M. Carr, G.S. Tschumper

COMP 294. Density functional theory and *ab initio* investigation of the detection properties of cyromazine. **Y. Tu**, Y. Tseng, M. Appell

COMP 295. Aromaticity-modulated hydrogen bonding (AMHB). C. Wu, **Y. Zhang**, J. Wu

COMP 296. Visualizing the origin of kinetic isotope effects with Python. **Z. Liu**, O. Ogba, D.J. O'Leary

COMP 297. TDDFT modeling of Ni-doped TiO2 using bulk-mimicking finite clusters. **A. Meyer**, P. Darapaneni, J.A. Dorman, K. Lopata

COMP 298. Predicting the converged limit of titania surface energies, geometries, and adsorption energies from a three-point exponential fit. **A.N. Carlson**, A.L. Gagliardi, J.C. Kern, E.S. Gawalt, J.D. Evanseck

COMP 299. Molecular simulations of bubble formation in metastable liquids. **B. Gonzalez**, C. Desgranges, J. Delhommelle

COMP 300. Computational study of copper-catalyzed atom transfer radical polymerization (Cu-ATRP) and catalyst discovery via virtual screening. **C. Fang**, K.D. Fiebre, X. Pan, K. Matyjaszewski, P. Liu

COMP 301. Molecular structures and energetics of palladium nanoclusters. **E. Lakner**, Z. Fang, R. Craciun, D.A. Dixon

COMP 302. Computational investigation of intermolecular interactions between functionalized single-walled carbon nanotubes and polyethylene terephthalate. **E.A. Vazquez Montelongo**, A. Rico-Campos, D. Aztatzi-Pluma, J.J. Alvarado, E.O. Castrejon-Gonzalez, G.A. Cisneros

COMP 303. Electronic decomposition analysis of substituted metal alkene and alkyne complexes. **E. Isaacson**, J. Scanlon

COMP 304. Computing the Schlenk equilibrium for thiophene Grignard reagents. **E. Curtis**, A. Vitek, P.M. Zimmerman

COMP 305. Electronic structure theory calculations for the study of CO_2 separation processes in polymeric membranes. **J. Townsend**, B.K. Long, T. Saito, K.D. Vogiatzis

COMP 306. Molecular simulation of transport of DNA grafted nanoparticle. **J. McLaughlin**, C. Desgranges, J. Delhommelle

COMP 307. Computational predictions of the hydrogenation catalytic activity of SSHC. **J.C. Plascencia**, C. Liu, A.K. Wilson, L.A. Curtiss

COMP 308. Relative energies of diastereomeric xanthene complexes for use in developing chiral sensors. **K. Nye**, C. Stephenson, S.A. Smith, D.H. Magers

COMP 309. Modeling optical properties of silver-gold core-shell nanoparticles using finite-difference time-domain. **M. Fleck**, H.T. Smith, K. Lopata

COMP 310. Withdrawn

COMP 311. Self-assembly of noncanonical DNA base pairs on *h*-BN monolayer. **N. Saikia**, R. Pandey

COMP 312. Theoretical evaluation of diffusion constants of supercritical/liquid ammonia by means of *ab initio* Effective Fragment Potential ver.2 – MD simulation. **N. Kuroki**, H. Mori

COMP 313. Soft crystal force field for elucidation of crystal-crystal phase transition of gold isocyanide complexes. **N. Nakayama**, S. Obata, H. Gotoh, T. Seki, H. Ito

COMP 314. Complexation energetics and thermodynamics of a CMPO-based chelator for selective lanthanide extraction from acidic solution. **O. Sode**

COMP 315. Computer simulations of polymers designed to detect polycyclic aromatic hydrocarbons. **P. Keck**

COMP 316. Electron-nuclear dynamics in the $[Au_{25}(SR)_{18}]^{-1}$ (R = H, CH_3, C_2H_5, C_3H_7, MPA), $Au_{18}(SH)_{14}$, and $Au_{38}(SH)_{24}$ nanoclusters: Ligand effects and size dependence. **R.D. Senanayake**, A.V. Akimov, C.M. Aikens

COMP 317. Influence of composition on

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the nucleation process in CuNi systems. **S. Bechelli**, C. Desgranges, J. Delhommelle

COMP 318. Assessing the environmental impact of energy production. **T. Komolafe**

COMP 319. Comprehensive study of the intramolecular interactions of unmethylated and methylated cyclodextrins using tight binding density functional theory and implicit solvent methods. M. Vazquez, **U. Schnupf**

Section A
Ernest N. Morial Convention Center
Hall E

NVIDIA GPU Award

M.E. Berger, C.L. Simmerling, *Organizers*

6:00–8:00

COMP 320. GPU molecular docking with convolutional neural network scoring functions. **J. Sunseri**, D. Koes

COMP 321. PMEMD 18: High performance molecular dynamics made accessible to scientific programming. **D.S. Cerutti**, D. Ghoreishi, S. Le Grand, A. Roitberg, R. Walker, D.A. Case

COMP 322. GPU-accelerated alchemical free energy simulations: A new tool for accurate, affordable prediction of ligand binding potency for drug discovery, optimization, and resistance problems. **T. Lee**, D.M. York

COMP 323. Investigating the dynamics of designed ligand-binding proteins. **E. Pecora de Barros**, R.E. Amaro

COMP 324. Accurate prediction of host-guest binding affinities via the AMOEBA force field. **M.L. Laury**, J.W. Ponder

Section A
Ernest N. Morial Convention Center
Hall E

OpenEye Outstanding Junior Faculty Award

C.L. Simmerling, *Organizer*

6:00–8:00

COMP 325. Simulating nanoscale energy and charge transport in soft molecular semiconductors. **A. Willard**

COMP 326. Curvature based lipid segregation and stability modulation in bilayers containing cardiolipin and monolysocardiolipin. K.J. Boyd, N.N. Alder, **E.R. May**

COMP 327. Constructing optimal structure-function relations directly from first principles. E. Berquist, K. Werling, **D. Lambrecht**

COMP 328. Strategies and software for accelerating inorganic molecular design. **H.J. Kulik**

Section A
Ernest N. Morial Convention Center
Hall E

Wiley Computers in Chemistry Outstanding Postdoc Award

M. Cavalleri, C.L. Simmerling, *Organizers*

6:00–8:00

COMP 329. Nuclear quantum effects successfully incorporated into nonadiabatic molecular dynamics dimulations *via* ring polymer surface hopping. **F.A. Shakib**, P. Huo

COMP 330. Embedded mean-field theory for high-efficiency electronic structure. **F. Ding**, F.R. Manby, T.F. Miller

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COMP and PMSE

WEDNESDAY MORNING

Section A
New Orleans Marriott Convention Center
New Levee

Material Science

1D & 2D Materials, Electron Transport & Opto-Electronic Properties

C.M. Aikens, *Organizer*
C. Sutton, *Presiding*

8:30 COMP 331. Interaction of carbon and boron nitride nanotubes with metals. **C. Rohmann**, D.J. Searles, M. Zwolak

8:55 COMP 332. Theoretical study of nitrogen-doped graphene nanoflakes: Stability and spectroscopic properties depending on dopant types and flake sizes. **C. Lin**

9:20 COMP 333. Inconsistencies in the electronic properties of phosphorene nanotubes: New insights from large-scale DFT calculations. **B.M. Wong**, S.I. Allec

9:45 COMP 334. TD-DFTB investigation of electronic structure and optical properties of silver nanorods and nanorod dimers. **F. Alkan**, C.M. Aikens

10:10 COMP 335. Ionic versus metallic nature of 2D electrides: A density-functional description. **S.G. Dale**, E.R. Johnson

10:35 Intermission.

10:50 COMP 336. Criticality of symmetry and decoherence in the photovoltaic properties of chalcogenide perovskites. **A. Nijamudheen**, A.V. Akimov

11:15 COMP 337. Simulations of charge transport in covalent organic frameworks. H. Kitoh-Nishioka, Y. Nishimoto, D.G. Fedorov, **S. Irle**

11:40 COMP 338. Computationally-driven development of OEO materials for nanoscale hybrid photonics. **L.E. Johnson**, A.F. Tillack, B. Robinson, L.R. Dalton, D.L. Elder

12:05 COMP 339. Towards novel organic electronics: Integrating simulation and neutron scattering. **T. Harrelson**, V. Dantanarayana, A. Santana Bonilla, A. Troisi, R. Faller, A.J. Moule

Section B
New Orleans Marriott Convention Center
River Bend 2

Drug Design

Algorithm, Tool & Web Service

Cosponsored by CINF
M.R. Landon, Y. Tseng, *Organizers*
P. Gupta, *Presiding*

8:30 COMP 340. Deep neural nets for predicting tyrosyl-DNA phosphodiesterase (Tdp1) potencies. **H. Sun**, Y. Wang, S. Michael

9:05 COMP 341. Design of property-biased chemical libraries using artificial intelligence approaches. M. Popova, O. Isayev, **A. Tropsha**

9:40 Intermission.

9:55 COMP 342. ProBiS tools at the PDB scale for drug discovery. **D. Janezic**, **J. Konc**

10:30 COMP 343. ProteinsPlus: Web-based computing at the interface of crystallography and structure-based design. S. Bietz, R. Fährrolfes, **M. Rarey**

11:05 COMP 344. Improving virtual screens with a new pharmacophore perception-scoring tool integrating MD of protein-ligand complexes. **K. Hauser**, M. Pierce, D.E. Watson, C.D. Von Bargen, S.L. Dixon, M.P. Repasky

Section C
New Orleans Marriott Convention Center
Julia

Quantum Mechanics

A.E. DePrince, *Organizer*
M. Piris, *Presiding*

8:30 COMP 345. Wavefunctions for strong correlation from exactly solvable models. **P.A. Johnson**

9:00 COMP 346. Using higher-order singular value decomposition to define weakly coupled and strongly correlated clusters: the *n*-body Tucker approximation. V. Abraham, **N. Mayhall**

9:30 COMP 347. Relativistic *ab initio* accurate minimal basis sets: Quantitative LUMOs and oriented quasi-atomic orbitals for the heavy elements. **G. Schoendorff**, A.C. West, M.W. Schmidt, K. Ruedenberg, M.S. Gordon

10:00 COMP 348. Deriving partial atomic charge from population analysis schemes: Effects of basis set quality and quantum mechanical approach. **K.R. Jorgensen**, A.K. Wilson

10:20 Intermission.

10:35 COMP 349. Even-handed active space selection in projection-based wavefunction-in-DFT embedding. **M. Welborn**, T.F. Miller

11:05 COMP 350. Modeling the absorption spectrum of charge-transfer chromophores in solution and in disordered aggregates. A. Kocherzhenko, J. Wilmer, A. Tillack, L.E. Johnson, B. Robinson, **C. Isborn**

11:35 COMP 351. Simulation of realistic electronic spectra band-shapes: The role of vibrational effects. **M. Biczysko**, J. Bloino

11:55 COMP 352. Perturbational molecular orbital approach for analyzing 3-center 2-electron bonds. **S. Bidwell**, H.P. Hratchian

Section D
New Orleans Marriott Convention Center
Blaine Kern D

Molecular Mechanics

Protein Stability, Folding & Design

M. Feig, *Organizer*
V.D. Cruzeiro, *Presiding*

8:30 COMP 353. Computational exploration of the β-grasp fold for structure, stability, and folding. **J. Bedford**, L.H. Greene, J. Poutsma

9:00 COMP 354. Protein folding, binding and aggregation in the cell: Role of stochastic resonance. **A. Davtyan**, G. Papoian

9:30 COMP 355. Intramolecular interaction in N-terminal regulatory region of c-Src kinase: A combined study of molecular dynamic simulation and small-angle scattering. **U.R. Shrestha**, P. Juneja, S. Pingali, Q. Zhang, J. Borreguero, V. Urban, H.M. O'Neill, J. Smith, L. Petridis

10:00 COMP 356. Insights into Ebola VP35 oligomerization from molecular simulations. **F. Di Palma**, V. Ramaswamy, G. Daino, A. Frau, A. Corona, L. Zinzula, E. Tramontano, P. Ruggerone, A.V. Vargiu

10:30 Intermission.

10:45 COMP 357. Effect of nucleotide state and salt concentration on the protofilament conformation of tubulin octamers. **A. Manandhar**, M. Kang, K. Chakraborty, S. Loverde

11:15 COMP 358. Stretching or heating proteins: Unravelling the molecular details of protein resistance to external perturbations. **G. Stirnemann**, S. Garcia-Manyes, F. Sterpone

11:45 COMP 359. Dehydrated DNA in B-form: Ionic liquids in rescue. **S. Senapati**

Section E
New Orleans Marriott Convention Center
Blaine Kern F

Structure-Based Drug Design for GPCRs
Cosponsored by CINF and MEDI
V. Shanmugasundaram, *Organizer*
Y. Che, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COMP 360. GPCR structures for drug discovery: The first decade and future perspectives. **X. Qiu**

9:05 COMP 361. Computational design of GPCR structure, stability and function. **P. Barth**

9:35 COMP 362. Unmasking full GPCR ligand design for potency, selectivity and kinetics from new and multiple ligand X-ray structures, water networks and GRID molecular interaction field analyses. **J.S. Mason**, F. DeFlorian, B.G. Tehan, G. Bottegoni, M. Congreve, F.H. Marshall

10:05 Intermission.

10:20 COMP 363. Structure-based

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screening for GPCR ligands from fragment and lead-like chemical space. **J. Carlsson**

10:50 COMP 364. *In silico* searches for selective small-molecule ligands of GPCRs with highly designed libraries. **P. Kolb**, F. Chevillard, D. Schmidt

11:20 COMP 365. Targeting GPR40 for diabetes: A multipronged approach. **J. Johnston**

11:50 COMP 366. Use of modeling and crystallography to understand CCR2 antagonist SAR and receptor binding. **A. Tebben**, P.H. Carter, R.J. Cherney

Adventures in Density Functional Theory

Materials & Molecular Modelling

Sponsored by PHYS, Cosponsored by COMP‡

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Sponsored by CATL, Cosponsored by COMP and ENFL

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Sponsored by PHYS, Cosponsored by COMP‡

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

WEDNESDAY AFTERNOON

Section A
New Orleans Marriott Convention Center
New Levee

Material Science

Materials Properties & Catalysis

C.M. Aikens, *Organizer*
O. Ozcelik, *Presiding*

1:30 COMP 367. Exploring doping in bulk chromia: Effects of dopant oxidation state on composition, vacancy defects and vacancy migration. **M. Nolan**, J. Carey

1:55 COMP 368. Density-functional study of the $La_2Zr_2O_7$ low-index surfaces. **Y.A. Mantz**, Y. Duan

2:20 COMP 369. Li-ion battery cathode materials and their computational characterization: A DFT investigation. **A. Abbaspour Tamijani**, D. Jones, J.W. Bennett, **S.E. Mason**

2:45 COMP 370. Influence of 5d transition-metal impurities on the thermoelastic properties of TiB_2: A first principle investigation. **M. Sun**, J. Liu

3:10 Intermission.

3:25 COMP 371. Computational design of defect-engineered $Ca(OH)_2$ monolayer for CO_2 capture. **O. Ozcelik**, K. Gong, C. White

3:50 COMP 372. Silicon carbide surfaces for pyrolysis studied with ReaxFF MD simulations. **T. Wei**

4:15 COMP 373. Unveiling the effect of Pt-based face-centered tetragonal core in core/shell nanoparticles for oxygen reduction reactions. **M. Liu**, H. Xin, D. Wang, Q. Wu

4:40 COMP 374. Amino acids conjugated gold clusters: Interaction of alanine and tryptophan with Au_8 and Au_{20}. M.H. Abdalmoneam, K. Waters, **N. Saikia**, R. Pandey

5:05 COMP 375. Molecular simulations of model bitumen compounds in solution and on clay mineral surfaces. **J. Mane**, S. Stoyanov

Section B
New Orleans Marriott Convention Center
River Bend 2

Drug Design

Molecular Dynamics

Cosponsored by CINF
M.R. Landon, Y. Tseng, *Organizers*
D. Janezic, *Presiding*

1:30 COMP 376. Understanding and designing cyclic peptides using molecular dynamics simulations and enhanced sampling methods. S. McHugh, D. Slough, H. Yu, J. Rogers, **Y. Lin**

2:00 COMP 377. Conformational insight into PRC2 mutation from molecular dynamics simulations. **T.M. Abramyan**, J.L. Suh, L.I. James, S.V. Frye, D. Kireev

2:30 COMP 378. Quantifying drug resistance at the atomic level through GPU-accelerated affinity simulations. **T. Lee**, D.M. York

3:00 Intermission.

3:15 COMP 379. Protein-ligand binding free energy calculations for challenging systems. **R. Abel**, L. Wang, H.S. Yu, W. Chen, E. Harder, Y. Deng, K. Borrelli

3:45 COMP 380. Application of free energy calculation methods to fragment-based drug discovery: Identification of new cyclophilin binders. **J. Michel**, C. Georgiou, H. Ioannidis, I. McNae, M. Wear, M. Walkinshaw

4:15 COMP 381. Towards *in silico* prediction of β-lactamase-mediated antibiotic resistance using free energy calculations. E. Selwa, E. Elisée, T. Naas, **B.I. Iorga**

4:45 COMP 382. Binding mode prediction and MD/MMPBSA-based free energy ranking for agonists of REV-ERBβ/NCoR. **Y. Westermaier**, S. Ruiz-Carmona, I. Theret, F. Perron Sierra, G. Poissonnet, C. Dacquet, J.A. Boutin, P. Ducrot, X. Barril

Section C
New Orleans Marriott Convention Center
Julia

Quantum Mechanics

A.E. DePrince, *Organizer*
E. Matito, *Presiding*

1:30 COMP 383. Efficient computational methods for studying electron detachment of metal oxide clusters. **H.P. Hratchian**

2:00 COMP 384. Performance of the Gaussian program on GPUs using the OpenACC programming model: Achieving a balanced, significant and affordable speed-up with respect to CPU-only architectures. **G. Scalmani**, R. Gomperts, M.J. Frisch, B. Leback

2:30 COMP 385. Closet-scale computing. **D. Matthews**

3:00 COMP 386. Development of a many-body carbon dioxide potential to explore the electronic and vibrational structure of gas and condensed phase CO_2. **O. Sode**

3:30 Intermission.

3:45 COMP 387. Maneuvering the challenges of QM calculations in biological contexts. **D.P. Harding**, A.N. Bootsma, S.E. Wheeler

4:05 COMP 388. Benchmarking the effective fragment potential dispersion correction to Hartree-Fock and density functional theory on the S22 test set. **S. Kim**, C. Kaliszewski, E. Guidez, M.S. Gordon

4:25 COMP 389. Modeling molecules in an interacting environment. **J. Charles**, S. Kais, T. Kubis

4:45 COMP 390. Parametrization and benchmark of the range separated LC-DFTB2 method for organic molecules. **V. Vuong**, J. Kuriappan, M. Kubillus, J. Kranz, T. Mast, T. Niehaus, S. Irle, M. Elstner

Section D
New Orleans Marriott Convention Center
Blaine Kern D

Molecular Mechanics

Binding & Recognition

M. Feig, *Organizer*
J.J. Karnes, *Presiding*

1:30 COMP 391. Deep cavity cavitand/alkane assembly state switching between monomeric and dimeric host:guest assemblies driven by guest packing. **D. Tang**, J.W. Barnett, B.C. Gibb, H. Ashbaugh

2:00 COMP 392. Molecular dynamics simulations of intracellular lipid binding proteins: Insights into ligand binding and water dynamics. N.H. Hunter, B. Bakula, E. Ellis, P. Koetting, **C.D. Bruce**

2:30 COMP 393. Binding of TMPyP4 to RNA G-quadruplex containing ALS and FTD related G4C2 repeat probed by all-atom molecular dynamics simulations with explicit solvent. **C. Wu**

3:00 COMP 394. Bidirectional allosteric modulation in *E. coli* glycinamide ribonucleotide transformylase (GAR Tfase). **P. Gupta**, A.E. Roitberg

3:30 Intermission.

3:45 COMP 395. Towards the rational design of alternative, eco-friendly herbicides targeting PSII. **H.P. Hendrickson**, H. Harrington, M. Jaladanki, V.S. Batista

4:15 COMP 396. Mechanism of molecular recognition in chemically distinct biomolecules. **T.J. Paul**, R. Prabhakar

4:45 COMP 397. Predicting site bound ions and water to nucleic acids using molecular solvation theory. **G.M. Giambasu**

Section E
New Orleans Marriott Convention Center
Blaine Kern F

Structure-Based Drug Design for GPCRs
Cosponsored by CINF and MEDI
Y. Che, *Organizer*
V. Shanmugasundaram, *Organizer, Presiding*

1:30 COMP 398. One receptor, many partners: How do GPCRs stimulate diverse signaling proteins? **R.O. Dror**

2:00 COMP 399. Structure-inspired design of β-arrestin-biased agonists for dopamine D2 receptor. **J. Jin**

2:30 COMP 400. Challenges and opportunities in structure-based discovery for GPCR targets and antitargets. **J. Karpiak**, D. Weiss, X. Huang, M.F. Sassano, B. Shoichet, B.L. Roth

3:00 Intermission.

3:15 COMP 401. Using forward and backward allostery in GPCRs to drug design. **N. Vaidehi**

3:45 COMP 402. Towards the development of improved painkillers to combat the opioid epidemics. **M. Filizola**

4:15 COMP 403. Intrinsic flexibility of the μ opioid receptor through multiscale modeling approaches. **D.P. Vercauteren**, M. Fosséprè, L. Leherte, A. Laaksonen

4:45 Concluding Remarks.

Adventures in Density Functional Theory

Excited States/Dynamics

Sponsored by PHYS, Cosponsored by COMP‡

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Sponsored by CATL, Cosponsored by COMP and ENFL

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Sponsored by PHYS, Cosponsored by COMP

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

THURSDAY MORNING

Section A
New Orleans Marriott Convention Center

‡*Cooperative Cosponsorship*

New Levee

Material Science

Thermodynamics, Statistical Mechanics & Dynamics

C.M. Aikens, *Organizer*
N. Saikia, *Presiding*

8:30 COMP 404. Modeling mechanisms and kinetics of phase transformations. **S. Andersson**, A. Lervik, Z. Wang, P. Xiao, I. Svenum, E. Riccardi, G.A. Henkelman, T.S. van Erp

8:55 COMP 405. Dynamical inversion of the energy landscape promotes non-equilibrium self-organization of binary particle mixtures. **L.A. Ruiz Pestana**, L.N. Lammers, T.L. Head-Gordon

9:20 COMP 406. Nucleation of capillary bridges and bubbles. C. Desgranges, **J. Delhommelle**

9:45 COMP 407. Finite size effects in simulations of molecular Joule-Thomson flow. **D. Rogers**

10:10 COMP 408. Modeling all recognized interactions of a supramolecular sensor and measurement designing to acquire genuine thermodynamic parameters. **F. Emami**

10:35 Intermission.

10:50 COMP 409. Structure and dynamics of self-assembled AAT nanotubes for siRNA-delivery. **T. Yu**

11:15 COMP 410. Influence of degree of functionalization on structural, thermodynamic and transport properties of anion exchange membrane: Insight from molecular dynamics simulations. **X. Wei**, D. Dong, D. Bedrov

11:40 COMP 411. Computer led design of functional arylamide foldamers part I: Towards selective water transport. **V. Pophristic**, Z. Liu, S. Makeneni, S. Houshyar azar

12:05 COMP 412. Molecular design of functionalized mesoporous silica nanoparticles for drug delivery applications. **A.A. Skelton**

Section B
New Orleans Marriott Convention Center
River Bend 2

Drug Design

Agonist, Antagonist & Macrocycle

Cosponsored by CINF
M.R. Landon, Y. Tseng, *Organizers*
S. Lenka, *Presiding*

9:00 COMP 413. Exploring the structural features of peripherally-restricted CB1 receptor antagonists and inverse agonists. **A. Aderibigbe**, P. Pandey, R.J. Doerksen

9:30 COMP 414. Accurate and reliable prediction of the binding affinities of macrocycles to their protein targets. **H. Yu**, Y. Deng, Y. Wu, D. Sindhikara, A. Rask, T. Kimura, R. Abel, L. Wang

10:00 Intermission.

10:15 COMP 415. Withdrawn

10:45 COMP 416. Challenges in the discovery of macrocyclic cyclophilin inhibitors. **U. Schmitz**, D. Shivakumar, B. Schultz, J. Paulsen, L. Wang, E. Harder, H.S. Yu, C. Higgs

11:15 COMP 417. Predicting targeted kinase inhibitor resistance to clinical Abl mutations using alchemical free-energy calculations. **K. Hauser**, C. Negron, S. Albanese, S. Ray, L. Wang, D. Lupyan, T.B. Steinbrecher, R. Abel, J.D. Chodera

Section C
New Orleans Marriott Convention Center
Julia

Quantum Mechanics

A.E. DePrince, *Organizer*
J.W. Hollett, *Presiding*

8:30 COMP 418. Extending the timescales of nonadiabatic molecular dynamics simulations. **A.V. Akimov**

9:00 COMP 419. Reaction mechanisms of benzylpenicillin acylation and deacylation with DD-peptidase. **Q. Cheng**, N.J. Deyonker

9:30 COMP 420. NAMD and VMD combined for easy and fast QM/MM simulations. **R.C. Bernardi**, M.C. Melo, K. Schulten, Z. Luthey-Schulten

9:50 COMP 421. Withdrawn

10:10 Intermission.

10:25 COMP 422. Withdrawn

10:45 COMP 423. Non-oxo complexes as oxygen transfer agents for oxidation of organic substrates. A computational study. **R. Parveen**, T.R. Cundari

11:05 COMP 424. Unraveling the nature of hydrogen bonds in pincer pyrazine Pd complexes with a quantum topological criterion. **E.A. Vazquez Montelongo**, J. Lohrman, H. Telikepalli, V. Day, M.A. Hix, K. Bowman-James, G.A. Cisneros

11:25 COMP 425. Theoretical investigations of simple carbohydrates by density-functional tight-binding: A comparative analysis to density functional theory. **K. Lee**, S. Irle, U. Schnupf

11:45 COMP 426. Diffusion Monte Carlo simulations of gas phase and adsorbed isotopically impure hydrogen clusters. **E. Curotto**, M. Mella

Section D
New Orleans Marriott Convention Center
Blaine Kern D

Molecular Mechanics

Polymers, Sugars & Foldamers

M. Feig, *Organizer*
R. Parveen, *Presiding*

8:30 COMP 427. Nonpolar solute cononsolvency in water/ethanol mixtures – Connections to solvent structure. **A. Saltzman**, H. Houser, M. Langrehr, H. Ashbaugh

9:00 COMP 428. Investigation of reverse osmosis membranes by weight-averaged anharmonic vibrational analysis. **D. Surblys**, T. Yamada, K. Yagi, Y. Sugita

9:30 COMP 429. Development progress in constructing atomic scale models of diverse lignins. **J.V. Vermaas**, L. Petridis, G. Beckham, M.F. Crowley

10:00 Intermission.

10:15 COMP 430. Computer led design of functional arylamide foldamers part II: Recognition and encapsulation of monosaccharide and sugar alcohols. **Z. Liu**, S. Makeneni, E.C. Fluck, V. Pophristic

10:45 COMP 431. Insights on the effects of point mutations at the dimer interface of *E. coli* β clamp from computational simulations. **H. Gokcan**, B. Koleva, P.J. Beuning, G. Cisneros

11:15 COMP 432. Withdrawn

Adventures in Density Functional Theory
Sponsored by PHYS, Cosponsored by COMP‡

THURSDAY AFTERNOON

Adventures in Density Functional Theory
Sponsored by PHYS, Cosponsored by COMP‡

ENFL

Division of Energy and Fuels

J. Liu, *Program Chair*

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 231

Materials & Processes for Solar Energy Conversion & Utilization

Y.H. Hu, R.T. Koodali, *Organizers*
B. Zhou, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 1. High efficient organic pollutants degradation and simultaneous electricity production based on solar photocatalytic initiation. **B. Zhou**

8:40 ENFL 2. 3D printing of patterned hybrid aerogel membrane for broadband solar wastewater purification. **H. Zhou**, T. Fan, D. Zhang

9:00 ENFL 3. CdS as holes provider for visible light-induced urea photo-oxidation. **R. Zhao**, J. Radich

9:20 ENFL 4. Identifying the mechanism of triplet pair separation in singlet fission through TIPS-pentacene polymorphs. **G. Doucette**, C. Grieco, E. Kennehan, J.B. Asbury

9:40 Intermission.

9:55 ENFL 5. Mediating the rates of singlet fission in 6,13-dipenylpentacene aggregates with PbS quantum dots. **C. Wang**, E. Weiss

10:15 ENFL 6. Sebacate anions intercalated NiFe layered double hydroxide as a high-performance electrocatalyst for oxygen evolution reaction. **Y. Dong**, S. Komarneni

10:35 ENFL 7. Phase change capsule with water-absorbable polymeric shell for thermal energy storage and delivery. **Y. Jung**, Y. Ko, T. Do

10:55 ENFL 8. Polaron formation mechanisms in conjugated polymers. **J. Bombile**, M.J. Janik, S. Milner

11:15 ENFL 9. Candelilla wax as renewable source for development of solar-thermal energy conversion and storage materials. L.G. Delgado-Interial, **C. Espinoza-González**, J.R. López-Muñoz, O.S. Rodriguez-Fernández, S. Fernández-Tavizón, J. Rodríguez-Hernández

11:35 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 232

Bioenergy & Bio-Based Chemicals
Cosponsored by CELL
J. Chang, S. Fu, *Organizers*
J. Fu, T. Morgan, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 ENFL 10. Renewable fuels from biomass-derived feedstocks: Opportunities and challenges. **A. Padmaperuma**, M.V. Olarte

8:55 ENFL 11. Biohydrogen production from switchgrass via pyrolysis-microbial electrolysis pathway. **A. Borole**, A. Lewis

9:20 ENFL 12. Redox-active renewable chemical feedstocks in agricultural commodities. **S.M. Uchimiya**

9:40 ENFL 13. Parametric study for the optimization of ionic liquid pretreatment of corn stover. **B.A. Simmons**, G. Papa, T. Feldman, K. Sale

10:00 Intermission.

10:15 ENFL 14. Constant-volume carbonization of biomass. **T. Morgan**, M.L. Arizaleta, S.Q. Turn, M.J. Antal, Ø. Skreiberg, W. Liang, M. Grønli

10:45 ENFL 15. Progress towards electrochemical processes for low-temperature and low-pressure bio-oil hydrogenation. **J. Holladay**, J. Lopez-Ruiz, U. Sanyal, J. Egbert, O.Y. Gutierrez-Tinoco, A.B. Padmaperuma

11:10 ENFL 16. Comparison of pyrolysis products yields derived from three different parts of poplar trees using a novel reactor. **D. Boldor**, C. Marculescu

11:35 ENFL 17. Computational insights to fuels and chemicals extraction from microbial biorefineries. **J.V. Vermaas**, G. Beckham, M.F. Crowley

11:55 ENFL 18. Hydrothermal liquefaction for marine macroalgal biorefinery. **S. Raikova**, C. Chuck, M. McManus, M.J. Allen

12:15 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 237

Materials & Processes for Solar Energy Conversion & Utilization

Y.H. Hu, *Organizer*
R.T. Koodali, *Organizer, Presiding*

‡*Cooperative Cosponsorship*

7:55 Introductory Remarks.

8:00 ENFL 19. Organic-inorganic hybrid perovskite deposition and passivation for high efficiency solar cells. T. Zhang, G. Li, F. Xu, **Y. Zhao**

8:30 ENFL 20. Optimizing multiple energy relay GUMBOS dyes for dye-sensitized solar cells. **T. Vargas-Myers**, P.E. Kolic, R.L. Perez, K.S. McCarter, I.M. Warner

8:50 ENFL 21. Effect of molecular electrolyte additives on photocurrent and photovoltage of dye-sensitized solar cells. **H. Cheema**, J.H. Delcamp

9:10 ENFL 22. Photon management in series-sequential multifunction dye-sensitized solar cells (SSM-DSC): Solar powered CO2 reduction coupled with water oxidation. **J.H. Delcamp**, H. Cheema, R.R. Rodrigues

9:30 ENFL 23. In-free thin-film solar cells: $Cu_2ZnSn(S,Se)_4$ films generated from a single molecular precursor solution. **D.J. Fermin**, D. Tiwari

9:50 Intermission.

10:05 ENFL 24. Investigation of charge carrier dynamics in organo-halide perovskites using time-resolved infrared spectroscopy. **K.T. Munson**, E.R. Kennehan, J.B. Asbury

10:25 ENFL 25. Electrochemistry and spectroelectrochemistry of lead halide perovskite films: Materials science aspects and boundary conditions. G.F. Samu, R.A. Scheidt, P.V. Kamat, **C. Janaky**

10:45 ENFL 26. Norbornadiene-quadricyclane photochromic systems for solar energy storage applications and testing in devices. **A. Dreos**, K. Jorner, K. Börjesson, Z. Wang, H. Ottosson, K. Moth-Poulsen

11:05 ENFL 27. Scatter function determination of high-temperature, inorganic oxide solar absorber coating morphology. **D. Karas**, A. Miller, J. Byun, J. Moon

11:25 ENFL 28. Interrogating exciton delocalization in films of peryelene diimides using ultrafast vibrational spectroscopy. **E. Kennehan**, C. Grieco, G. Doucette

11:45 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 239

Natural Gas Catalysis

J. Baltrusaitis, K. Ding, N. Kumar, *Organizers*
J.J. Spivey, *Organizer, Presiding*
K. Ding, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 29. *In situ* investigation of methane dry reforming on M-CeO_2 {M= Co, Ni, Cu} catalysts: Metal-support interactions and the activation of C-H bonds at room temperature. **J. Rodriguez**

8:40 ENFL 30. Stabilizing catalysts for dry reforming of methane. P. Littlewood, **P.C. Stair**

9:20 ENFL 31. Hydrotalcite-zirconia composite as co-catalyst for the dry reforming of methane. **A.P. Tathod**, O. Gazit

9:40 Intermission.

9:55 ENFL 32. Activity and mechanism of methane oxidation over Pd/Al_2O_3 catalyst. **A.C. Banerjee**, J. McGuire

10:15 ENFL 33. Kinetic investigation of methane partial oxidation at high pressure over Ni-substituted hexaaluminate catalysts. **T.H. Gardner**

10:35 ENFL 34. Effect of temperature in methane activation using $AlBr_3$ supported H-ZSM-5 catalysts. **S. Kanitkar**, N. Kumar, Z. Wang, J. Carter, K. Ding, G. Hutchings, J.J. Spivey

10:55 ENFL 35. Low temperature selective methane oxidation to methanol utilizing molecular oxygen with gold palladium colloidal catalysts. N. Agarwal, S. Freakley, R.U. McVicker, S.M. Althahban, N. Dimitratos, Q. He, D.J. Morgan, D.J. Willock, S.H. Taylor, C. Kiely, **G. Hutchings**

11:35 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 240

Advanced Analytical Techniques for Determination of Minor & Trace Elements in Petroleum Value Chain

J. Casey, C.S. Hsu, F.A. Lopez-Linares, *Organizers*
J. Nelson, *Organizer, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 36. Determination of HgS nanoparticles in produced water by single particle inductively coupled plasma spectroscopy (sp-ICP-MS). **J. Nelson**

8:30 ENFL 37. Single reaction chamber microwave sample preparation for determination of 57 major, minor, trace and ultra-trace elements and V, Fe and S stable isotope ratios for unambiguous fingerprints of crude and refined oils, by-products, extractable organic material, kerogen and source rocks. **J. Casey**, Y. Gao, T. Sun, K. Bissada

8:55 ENFL 38. Analysis of distillate products per ASTM D8110-17 using the Agilent 7800 and Teledyne-Cetac MVX-7100 uL autosampler. **L. Whitecotton**

9:20 ENFL 39. Dynamic headspace analysis – Hg speciation in petroleum hydrocarbons just got cleaner. **Z. Gajdosechova**, Z. Mester, E. Pagliano

9:45 Intermission.

10:00 ENFL 40. Measurement of metal carbonyls in carbon monoxide and fuels containing carbon monoxide by GC-ICP-MS. **W. Geiger**

10:25 ENFL 41. Characterization of ultradispersed catalysts in heavy oil fractions by single particle inductively coupled plasma-triple quadrupole mass spectrometry (sp-ICP-MS/MS). J. Nelson, M. Yamanaka, V. Rodriguez-DeVecchis, L.A. Carbognani, P. Pereira-Almao, **F.A. Lopez-Linares**

10:50 ENFL 42. Heteroatom incorporation during MFI crystallization as measured by single particle inductively coupled plasma mass spectrometry. **T. Davis**, J. Nelson

11:15 ENFL 43. Using AF4-ICP-MS, sp-ICP-MS and TEM for the characterization of Hg-containing nanoparticles in gas condensate samples. **D. Ruhland**, K. Nwoko, M. Perez, J. Feldmann, E. Krupp

11:40 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 241

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
H. Chen, F. Lin, K.A. See, *Organizers*
Y. Mo, *Organizer, Presiding*
Y. Yan, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 44. "Burning" lithium in CS_2: Compact Li_2S@graphene nanocapsules for Li-S batteries. **J. Lu**

8:30 ENFL 45. Crosslinked disulfide polymers suppress polysulfide shuttle in Li–S batteries. **M. Preefer**, B.D. Oschmann, C.J. Hawker, R. Seshadri, F. Wudl

8:50 ENFL 46. Dynamics structure of the buried functional interface in an advanced lithium/sulfur cell. **T. Pascal**

9:10 ENFL 47. Lock sulfur in confined nanostructures to improve the performance of Li-S batteries. Y. Pei, N. Baxter, Y. Wang, **S. Wang**

9:30 Intermission.

9:50 ENFL 48. Molecular ionic composite electrolytes to enable safer and higher energy density batteries. **L.A. Madsen**, Y. Wang, C. Zanelotti, S.E. Wollman, D. Yu, Y. He, Z. Yu, R.J. Fox, R. Kerr, M. Forsyth, R. Qiao, T.J. Dingemans

10:20 ENFL 49. Nanostructuring at the interface for efficient and high capacity-performing free standing electrodes in all solid-state Li-S batteries. H. El-Shinawi, E. Cussen, **S. Corr**

10:40 ENFL 50. *Ab initio* studies of solvation effects in sparingly solvating electrolytes for lithium-sulfur batteries. **B. Narayanan**, R. Assary, M. Shin, T.S. Watkins, H. Wu, K.A. See, L. Zhu, R.T. Haasch, S. Zhang, Z. Zhang, A.A. Gewirth, K.R. Zavadil, L.A. Curtiss

11:00 ENFL 51. Understanding the role of solvent and added water on the effectiveness of lithium iodide as a redox mediator in lithium oxygen batteries. **G. Leverick**, Y. Shao-Horn

11:20 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 238

Remediation of Wastewater from Energy Usage

Water Remediation & Produced Water

Y. Li, J. Ren, *Organizers*
T. Atesin, *Presiding*

8:25 Introductory Remarks.

8:30 ENFL 52. Efficient removal of ultrafine coal particles from power plant effluent streams using flocculation-sedimentation-filtration process. A. Bhagavatula, V. Rajagopalan, **B. Duncan**, P. Vimalchand, M. Nelson

8:55 ENFL 53. Degradation of model naphthenic acids and naphthenic acids in oil sands process-affected water (OSPW) by UV activated persulfate method. **F. Zhi**, R. Huang, P.C. Ayala, Q. Shi, C. Xu, M.G. El Din

9:20 ENFL 54. Theoretical comparison of DCMD and VMD for desalination of high salinity wastewaters. **O.R. Lokare**, R.D. Vidic

9:45 ENFL 55. Non-catalytically intensify continuous production of biodiesel from microalgae by extraction coupling with transesterification under supercritical conditions. **J. Yin**, B. Qiao, D. Zhou, Q. Xu

10:10 Intermission.

10:25 ENFL 56. Visible-light-driven photocatalytic degradation of organic water pollutants promoted by sulfite. **W. Deng**, Y. Li

10:50 ENFL 57. Energetic and techno-economic comparison of mechanical vapor recompression and direct contact membrane distillation for shale gas produced water desalination. **E. Shamlou**, S. Tavakkoli, O.R. Lokare, R.D. Vidic, V. Khanna

11:15 ENFL 58. Use of microbial electrolysis cells for produced water treatment. **A. Borole**, S. Satinover, C. Tsouris

11:40 Concluding Remarks.

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL and PHYS

Wood-Based Materials for Energy & Water

Nanocellulose-Based Technologies

Sponsored by CELL, Cosponsored by ENFL, ENVR and MPPG

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 231

Bioenergy & Bio-Based Chemicals

‡*Cooperative Cosponsorship*

Cosponsored by CELL
J. Chang, S. Fu, *Organizers*
J. Fu, T. Morgan, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 59. Biofuel and biorenewables from the *carinata* biomill. **S.A. Miller**, S. Shen

1:55 ENFL 60. Synergy between woody biomass and scrap tyre upon co-pyrolysis for the production of bio-oil. T. Jayasinhe, A. Zarei, A. De Girolamo, **L. Zhang**

2:20 ENFL 61. Identification of sulfur-containing impurities in fatty acid methyl esters produced from brown grease. **V.T. Wyatt**, K. Jones, M. Hughes, M.E. Hums, R. Cairncross

2:45 ENFL 62. Oxidation stability of biodiesel derived from waste catfish oil. **J. Fu**, S.Q. Turn, B.T. Hue, P. Le

3:10 Intermission.

3:25 ENFL 63. Alternative jet fuel production from tropical biomass resources. **T. Morgan**, S.Q. Turn

3:55 ENFL 64. Future, feedstock agnostic, biorefineries for the production of lipid and higher value products through an integrated microwave and biological process. **C. Chuck**, J. Clark, A. Fan, F. Santomauro, V. Budarin

4:15 ENFL 65. Systematic analysis of cloud points and crystallization in fatty acid ethyl ester biodiesel mixtures with and without additives. P. Leggieri, **M. Senra**, L. Soh

4:35 ENFL 66. Effects of bentonite based catalyst on conversion of rapeseed oil to methyl esters via reactive separation. B. Ali, **S. Yusup**, A. Quitain, R. Kamil, T. Kida, A. Bokhari

4:55 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 232

Carbon Dioxide Conversion & Artificial Photosynthesis
Cosponsored by CATL, COMP and GEOC
Y.H. Hu, H. Lin, C. Liu, *Organizers*
S. Kawi, *Organizer, Presiding*
H. Zhou, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 67. Preparation aspects of coke resistance nickel catalyst for CO_2 reforming of methane. **Q. Li**

1:55 ENFL 68. Nanostructured catalysts for carbon dioxide conversion. Z. Wang, Y. Guo, **Y. Fang**

2:20 ENFL 69. CO_2 reforming of methane over Ni-based catalyst. **S. Wang**, Y. Lu, Y. Zhao, X. Ma

2:45 ENFL 70. Kinetic and mechanistic insights for CO_2-H_2O reforming of methane over Ni-phyllosilicate structure derived Ni-SiO_2-MgO catalysts. **A. Jangam**, S. Kawi

3:10 Intermission.

3:25 ENFL 71. CO2 activation and methanation on Ni-modified metal oxides: Insights from experiment and modelling. **M. Nolan**, A. Van Veen, M. Li

3:50 ENFL 72. Conversion of CO_2 into multi-products via the molybdenum alkoxide catalyst. J. Chen, **J. Ma**, P. Cheng

4:15 ENFL 73. Improving CO_2 capture performance by incorporating functionalized materials into porous polymer networks. **G.S. Day**, M.R. Bosch, J.A. Willman, E.A. Joseph, H. Drake, K. Ozdemir, H. Zhou

4:40 ENFL 74. Theoretical insights into supported metal catalysts for highly selective CO_2-to-CO conversion. **X. Su**, X. Chen, H. Su, Y. Huang, T. Zhang

5:05 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 237

Materials & Processes for Solar Energy Conversion & Utilization

R.T. Koodali, *Organizer*
Y.H. Hu, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 75. Synthesis and photocatalytic application of ultrastable core/shell quantum dots. **L. Liang**, L. Kong, Z. Li

2:00 ENFL 76. Semiconductor photocatalysis of bicarbonate to solar fuels: Formate production from copper (I) oxide. **H. Pan**, S. Chowdhury, M. Heagy

2:20 ENFL 77. Charge carrier recombination in anatase and rutile TiO_2 single crystals: Role of defects and hydrogen production. **K. Katsiev**, P. Maity, H. Ghamdi, O. Mohammed, H. Idriss

2:40 ENFL 78. Photocatalytic hydrogen generation activity at plasmonic Au–TiO_2 and Au–TiO_2/Pt aerogels. **J. Pietron**, P. DeSario, T.H. Brintlinger, A. Dunkelberger, O.A. Baturina, J. Owrutsky, D.R. Rolison

3:00 ENFL 79. CuO_x-TiO_2 composite photocatalysts for photocatalytic H_2 production. **W. Huang**

3:20 Intermission.

3:35 ENFL 80. Spin-dependent photoinduced electron transfer in a prototype artificial-photosynthesis molecular framework. **S. Hedstrom**, S. Chaudhuri, N.T. La Porte, M.R. Wasielewski, V.S. Batista

3:55 ENFL 81. Sprayed CZTS photoelectrode from stable precursor solution & study of charge transfer dynamics. **A. Mondal**, J. Radich

4:15 ENFL 82. Synthesis, photocatalytic properties and Langmuir-Blodgett film: Photoelectrochemical behavior of CdS and CdSe nanoparticles of hydrophilic or hydrophobic organic shell. **M. Nagamine**, M. Osial, P. Krysinski, J. Widera

4:35 ENFL 83. High efficiency luminescent solar concentrating devices using copper-indium-sulfide quantum dot nanocomposite laminated glass. **A. Jackson**, K. Ramasamy, M. Bergren, N. Markarov, H. McDaniel

4:55 ENFL 84. Chlorinated π-conjugated polymer with efficiency over 11% and enhanced stability in organic solar cells. **F. He**

5:15 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 239

Natural Gas Catalysis

J. Baltrusaitis, K. Ding, N. Kumar, *Organizers*
J.J. Spivey, *Organizer, Presiding*
K. Ding, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 85. Transformation of lower alkanes by oxygen in the presence of HCl catalyzed by modified CeO_2 nanocrystals. Q. Xie, H. Zhang, J. Kang, Q. Zhang, **Y. Wang**

2:10 ENFL 86. Aromatization of C2-C3 molecules to benzene-related molecules. **F. Tao**

2:50 ENFL 87. Microwave-assisted conversion of low rank coal under methane environment. **V. Abdelsayed**, D. Shekhawat, M. Smith, S. Hammache

3:10 ENFL 88. Fischer-Tropsch synthesis: Improved conversion and selectivity with Co/silica by foregoing calcination and utilizing reduction promoters. **M. Mehrbod**, G. Jacobs, M. Martinelli, B.H. Davis, D.C. Cronauer, A.J. Kropf, C.L. Marshall

3:30 ENFL 89. Rate and mechanism of oxidative coupling of methane over hydroxyapatite-based catalysts. **D. Liu**, S. Oh

4:10 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 240

Shale Gas Extraction, Conversion & Utilization

L. Fan, F. Li, *Organizers*
L. Neal, T. Wang, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 90. Process intensification technologies for natural gas upgrading. **G. Veser**

2:10 ENFL 91. Olefin production from natural gas condensates using a cyclic redox scheme. **L. Neal**, V. Haribal, F. Li

2:50 ENFL 92. Effective methods for treating and recycling produced water in unconventional oil operations. **M.A. Reynolds**, E.E. Hansen, S. Leung

3:40 Intermission.

3:55 ENFL 93. Analysis of the effectiveness of different injection fluids in huff-and-puff method of enhanced hydrocarbon recovery in shale fracture networks using microfluidic experiments. **P. Nguyen**, B. Carey, M. Porter, H. Viswanathan, J. Sheng

4:25 ENFL 94. Novel microbial biosensor platforms for early detection and treatment of oil leakage and produced waters. **V. Gude**, H. Nandimandalam

4:55 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 241

Advanced Analytical Techniques for Determination of Minor & Trace Elements in Petroleum Value Chain

J. Casey, C.S. Hsu, F.A. Lopez-Linares, *Organizers*
J. Nelson, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 95. How far can we go with LIBS for the fuel industry? **C. Lienemann**, F. Trichard, P. Dufresne, P. Galliou, W. Weiss, N. Gilon, V. Motto-Ros, F. Baco-Antoniali, L. Sorbier

2:10 ENFL 96. Trace metal analysis in fuels by MP-AES. **T. Alleman**, E. Christensen, L. Fouts

2:40 ENFL 97. Proposed ASTM method on elemental analysis of crude oil by microwave plasma atomic emission spectrometry (MP-AES). **N. Drvodelic**

3:10 Intermission.

3:25 ENFL 98. New ASTM ICPMS method in crudes. **J. Nelson**

4:05 ENFL 99. Molecular composition analysis of lubricant base oils by using RICO redox derivatization followed by ESI FT-ICR MS. M. Sutian, C.S. Hsu, **Y. Zhou**, Q. Shi

4:35 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 238

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
F. Lin, Y. Mo, K.A. See, *Organizers*
H. Chen, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 100. Sodium-sulfur flow battery for low-cost electrical storage. **Z. Li**

2:00 ENFL 101. Design of stable, high energy pyridine derived molecules for applications in redox flow batteries. **M.E. Cook**, J. Ruchti, M.S. Sanford, M.S. Sigman, S.D. Minteer

2:20 ENFL 102. Surface functionalization of silica (SiO_2) nanoparticles in Nafion nanocomposite membranes for vanadium redox flow batteries. **A.B. Jansto**, E. Davis

2:40 ENFL 103. Understanding the pseudocapacitive mechanism of MXene electrode in H_2SO_4 from joint density functional theory. **C. Zhan**, M. Naguib, M. Lukatskaya, P. Kent, Y. Gogotsi, D. Jiang

3:00 Intermission.

3:15 ENFL 104. Tannic acid-decorated spongy graphene for flexible and high performance supercapacitors. **L. Xu**, X. Jin

3:35 ENFL 105. Bacteria promoted 3D-nanotube structure for supercapacitor applications. **S. Ozden**, I. Macwan, P. Owuor, S. Kosolwattana, C. Tiwary, P. Autreto, R. Vajtai, A. Mohite, P. Patra, P. Ajayan

3:55 ENFL 106. Hollow carbon nanotubes templated from La_2O_3 nanorods as an electric double layer capacitor. **A.T. Brown**, Z. Wang, K.J. Balkus

‡*Cooperative Cosponsorship*

4:15 ENFL 107. Immiscible polymer blends to shepherd metal oxide precursors into carbon nanofibers. **J.A. Garcia**, S. Malekpour, K.J. Balkus, J.P. Ferraris

4:35 ENFL 108. Sputtered iridium oxide micro-supercapacitors operating in physiological environment with high energy density and cycle stability. **J. Maeng**, S.F. Cogan

4:55 ENFL 109. High yield bottom-up PECVD synthesis of graphene nanoribbons and their application in supercapacitors. **J. Bagley**, C. Hsu, W. Tseng, M.L. Teague, N. Yeh

5:15 Concluding Remarks.

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP‡, ENFL‡ and PHYS

Magnetically Recoverable Catalysts
Sponsored by CATL, Cosponsored by COLL, ENFL and INOR

Wood-Based Materials for Energy & Water

Wood-Fiber & Wood-Scaffold Based Technologies

Sponsored by CELL, Cosponsored by ENFL, ENVR and MPPG

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 231

ENFL Plenary: Reaction Mechanisms in Novel Energy & Fuel Conversion Systems

L. Fan, *Organizer*
R.T. Koodali, A.A. Park, *Presiding*

10:00 Panel Discussion.

10:00 ENFL 110. Strategies for the conversion of renewable carbon sources to fuels: Implications for catalysis. **A.T. Bell**

11:00 ENFL 111. Chemical looping technology for combustion, gasification, reforming, and chemical syntheses: Redox reaction mechanism and technology commercialization readiness. **L. Fan**

Section B
Ernest N. Morial Convention Center
Room 232

Carbon Dioxide Conversion & Artificial Photosynthesis

Theoretical Studies, Policy & Catalytic Conversion

Cosponsored by CATL, COMP and GEOC
Y.H. Hu, H. Lin, C. Liu, *Organizers*
S. Kawi, *Organizer, Presiding*
H. Zhou, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 112. Mechanistic insights into the synthesis of higher alcohols from syngas on CuCo-alloys. **A. Cao**, J. Schumann, F. Abild-Pedersen, Y. Liu, J.K. Norskov

8:25 ENFL 113. Activation and hydrogenation of CO_2 over iron carbide and oxide catalysts: Insight from DFT. **H. Wang**, X. Nie, X. Guo, C. Song

8:50 ENFL 114. New computational approach to determine the role of vibrational kinetics in low temperature plasmas used for CO_2 dissociation. **R. Van de Sanden**, S. Longo, P. Diomede

9:15 ENFL 115. Theoretical insights for low-overpotential electroreduction of CO_2/CO on Cu surfaces. **L. Cao**, T. Mueller

9:35 ENFL 116. Nanocrystalline Co(II) metal-organic framework for the conversion of CO_2 into cyclic carbonates. **P. Cheng**, X. Ji, J. Ma

9:55 Intermission.

10:05 ENFL 117. CO_2 utilization: A view from China National Petroleum Corporation. **J. Hu**

10:30 ENFL 118. Withdrawn

10:50 ENFL 119. Bicarbonate hydrogenation by iron: Effects of solvent and ligand on the mechanism. **M. Ahlquist**, R. Marcos

11:10 ENFL 120. Using CO_2 and CH_4 as C1 building blocks to produce value-added product through C-C coupling. Y. Zhao, H. Wang, X. Zhu, J. Han, **Q. Ge**

11:30 ENFL 121. Advances in studies of structural effect of Ni catalysts for CO_2 conversion. **C. Liu**

Section C
Ernest N. Morial Convention Center
Room 237

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
H. Chen, Y. Mo, K.A. See, *Organizers*
F. Lin, *Organizer, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 122. Hierarchical design of a novel Cu/Ni/TiO_2 electrode for lithium-ion batteries. **Y. Yue**, H. Liang

8:20 ENFL 123. Nitrogen-deficient graphitic carbon nitride for Li-ion battery anode applications. J. Chen, Z. Mao, D. Wang, L. Bie, **B.D. Fahlman**

8:40 ENFL 124. Electrodeposition of high energy density anodes for rechargeable batteries: Unusual anode-substrate interactions. M.C. Schulze, E.D. Jackson, J. Ma, **A.L. Prieto**

9:10 ENFL 125. BIAN based conjugated polymer binder for Li ion secondary battery anodes. **S.G. Patnaik**, R. Vedarajan, N. Matsumi

9:30 ENFL 126. Studying the rate of electron transfer at pyrolytic carbon electrodes. **J.C. Lytle**, G.E. Kamm, T. Le, E.M. Ness, J.F. Parker, D.R. Rolison, J.W. Long

9:50 Intermission.

10:05 ENFL 127. Structural engineering of two-dimensional nanomaterials for efficient energy storage. Y. Zhu, **G. Yu**

10:35 ENFL 128. Continuous synthesis of graphene oxide materials in a model Taylor-Couette flow reactor. **M. AlAmer**, Y.L. Joo

10:55 ENFL 129. Holey graphene for electrochemical energy storage. **R. Kanungo**, J. Radich

11:15 ENFL 130. Highly stable two and three lithium insertion in amorphous V_2O_5 shells coaxially deposited on electrospun carbon nanofibers: A self-supported membrane for high-capacity lithium ion battery cathodes. **J.E. Brown**, J. Li

11:35 ENFL 131. *Operando* Bragg coherent x-ray diffraction investigation of transformations in individual alloying anode particles. **F.J. Cortes**, M.G. Boebinger, M. Xu, A. Ulvestad, M.T. McDowell

Section D
Ernest N. Morial Convention Center
Room 239

Shale Gas Extraction, Conversion & Utilization

L. Fan, F. Li, L. Neal, T. Wang, *Organizers*
M. Zhao, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 132. *Bottoms-up* synthesis of commodity chemicals from shale gas. A. Chakrabarti, A. Wang, L. Sharma, G. Yan, J. Baltrusaitis, **I.E. Wachs**

8:50 ENFL 133. Functional materials for hydrogen production from shale gas reforming. G. Ji, M. Memon, **M. Zhao**

9:30 ENFL 134. Alkali-promoted mixed oxide redox catalysts for chemical looping-oxidative dehydrogenation of ethane (CL-ODH). **Y. Gao**, L. Neal, F. Li

10:10 Intermission.

10:25 ENFL 135. Catalytic conversion of light hydrocarbon gases to drop-in fuels using tri-reforming and hydrocarbon synthesis. X. Zhao, D. Walker, T. Roberge, B. Joseph, **J. Kuhn**

11:05 ENFL 136. Rh promoted perovskites as effective redox catalysts for chemical looping reforming of methane. **A. Mishra**, A. Shafiefarhood, F. Li

11:30 ENFL 137. Role of oxygen vacancies in oxidative coupling of methane over Mg_6MnO_8-based catalytic oxygen carriers in a chemical looping system. **S. Nadgouda**, D. Baser, L. Qin, Z. Cheng, L. Fan

Section E
Ernest N. Morial Convention Center
Room 240

Road Map & Policy of Energy & Fuels

Reducing America's Carbon Footprint through Nuclear Energy: Policy Perspectives & Other Non-Nuclear Technologies & Practices

Cosponsored by ENFL
S. Liu, Q. Zhen, *Organizers*
S. Bashir, C. Sanders, M. Sanders, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 138. Reducing America's carbon footprint through nuclear energy: Framework of the debate over nuclear energy. **M. Sanders**, **C. Sanders**

8:30 ENFL 139. Reducing America's carbon footprint through nuclear energy: Historical development related to risk assessment and potential methods. **M. Sanders**, **C. Sanders**

9:00 ENFL 140. Reducing America's carbon footprint through nuclear energy: Assessment of safety and measured criteria. **M. Sanders**, **C. Sanders**

9:30 ENFL 141. Reducing America's carbon footprint through nuclear energy: Viable energy source for power generation. **M. Sanders**, **C. Sanders**

10:00 Intermission.

10:15 ENFL 142. Can parked cars and carbon taxes create a profit? The economics of vehicle-to-grid energy storage for peak reduction. G. Freeman, H. Gandhi, **A. White**

10:40 ENFL 143. Synthesis of high-density fuels from biomass derivatives. **J. Xie**, G. Nie, X. Zhang, J. Zou

11:05 ENFL 144. Study of deposition behavoir of asphaltenes sub-fraction with microfluidic system. **T. Cao**, Y. Lin, A. Yen, S. Biswal, J. Macias

11:30 ENFL 145. Computational and experimental study of CO_2 capture by alkylamines. **K. Yang**, J. Schell, R. Glaser

Section F
Ernest N. Morial Convention Center
Room 241

Hydrogen Energy: Production, Storage & Application

T. Autrey, V. Stavila, *Organizers, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 146. U.S. Department of Energy activities in hydrogen production, delivery, and storage. **Z. Hulvey**, K. Randolph, N. Stetson

8:20 ENFL 147. Unravelling the mechanism of complex metal hydride reversibility by catalytic metal sites. **M. Allendorf**, H. Bluhm, F. El Gabalay, J. Guo, R.D. Kolasinski, Y. Li, T. Ogitsu, A.J. Rowberg, V. Stavila, J.L. White, J.A. Whaley, B. Wood

8:40 ENFL 148. Hydrogen storage characterization and optimization research effort, HySCORE. **T. Gennett**, P. Parilla

9:00 ENFL 149. Neutron measurements of hydrogen storage materials. **C.M. Brown**, T.J. Udovic, J. Tarver

9:20 ENFL 150. Characterization, optimisation and perspectives of light weight metal hydride materials and systems based thereon for hydrogen storage. **M. Dornheim**

9:40 Intermission.

‡*Cooperative Cosponsorship*

9:55 ENFL 151. Synthesis and reactivity of potassium octahydrotriborate salt. **X. Chen**, X. Chen, J. Wang, X. Feng, C. Cui, Y. Liang

10:15 ENFL 152. Study of molecular hydrogen at kbar pressures using inelastic neutron scattering and the case of hydrogen in Mg(BH4)2. **A. Ramirez-Cuesta**, L.L. Daemen, Y. Cheng

10:35 ENFL 153. Novel tools for the characterisation of hydrogenous materials. **M. Jones**

10:55 ENFL 154. Mesoporous carbons for the nano-confinement of hydrogen storage materials. **R. Janot**

11:15 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 238

Issues & Challenges Related to Heavy, Light & Shale Oil Production & Processing

J.J. Adams, P. Rahimi, Y. Zhang, *Organizers*
C.F. Ovalles, *Organizer, Presiding*
Y. Zhang, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 155. Asphaltenes, what art thou? **M.E. Moir**

8:25 ENFL 156. Imaging single molecules by scanning probe microscopy. **B. Schuler**

8:50 ENFL 157. Evidence for dominane of island architecture for asphaltenes. **O.C. Mullins**

9:15 ENFL 158. Non-contact atomic force microscopy (NC-AFM) imaging of asphaltene model compounds. **Y. Zhang**, M. Harper, D. Kushnerick

9:40 Intermission.

9:50 ENFL 159. Molecular structure of heavy oil revealed with non-contact atomic force microscopy. **Y. Zhang**, M. Harper, D. Kushnerick

10:15 ENFL 160. Asphaltenes are comprised of abundant island and archipelago structural motifs: A mass spec lesson in selective ionization. **R.P. Rodgers**, S. Rowland, M.L. Chacón-Patiño

10:40 ENFL 161. Heteroatom compositions and chemistry of petroleum system. **K. Qian**

11:05 ENFL 162. Ultrahigh purity vanadyl petroporphyrins. B.M. Rytting, **P.K. Kilpatrick**, I. Singh, M. Harper, A.S. Mennito, Y. Zhang

11:30 ENFL 163. Ultra small-angle X-ray scattering (USAXS) assessment of asphaltene precipitation and inhibitor effectiveness. **M. Hoepfner**, M. Ismail, Y. Yang, C.F. Ovalles, E. Rogel, M.E. Moir

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

***Operando* Techniques for Catalytic & Photocatalytic Fuel Conversion Studies**
Sponsored by CATL, Cosponsored by ENFL

Wood-Based Materials for Energy & Water

Wood-Based & Related Materials

Sponsored by CELL, Cosponsored by ENFL, ENVR and MPPG

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL and PHYS

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 231

Issues & Challenges Related to Heavy, Light & Shale Oil Production & Processing

C.F. Ovalles, P. Rahimi, Y. Zhang, *Organizers*
J.J. Adams, *Organizer, Presiding*
P. Rahimi, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 164. Study on wax deposition inhibitors. **J.J. Adams**, F.F. Tort, J.F. Schabron

1:55 ENFL 165. Effect of comb copolymers on flow ability of waxy oil under high pressure. **X. Guo**, T. Li, J. Xu, R. Zou, L. Li

2:20 ENFL 166. Identification of continuous chemical treatment products to manage paraffin deposition in the oilfield. **C. Russell**, E. Pohl, R. Sharpe

2:45 ENFL 167. Oilfield paraffin management: Novel test method development for the design of remediation chemical treatments. **C. Russell**, E. Pohl, R. Sharpe

3:10 Intermission.

3:25 ENFL 168. Asphaltenes wash off using terpene microemulsions. **H.W. Hernandez**, A. Perrard, P. Ashcraft, S. Trabelsi

3:50 ENFL 169. Analysis of fouling deposits. **E. Rogel**, K. Hench, G. Dickakian

4:15 ENFL 170. Investigating the relationship between vanadium content and viscosity of Athabasca bitumen during low temperature visbreaking: Role of the VO^{2+} ion. **K. Sivaramakrishnan**, G. Chauhan, A. De Klerk, V. Prasad

4:40 ENFL 171. Effects of self-assembly of paraffin on the transport property and viscosity of waxy crude oil. **X. Chen**, L. Hou, W. Li, D. Bedrov

5:05 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 232

Carbon Dioxide Conversion & Artificial Photosynthesis
Cosponsored by CATL, COMP and GEOC
Y.H. Hu, S. Kawi, H. Lin, C. Liu, *Organizers*
M. Liu, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 172. Electrocatalytic CO_2 reduction with nickel complexes supported by tunable macrocyclic bipyridyl-NHC ligands. **X. Su**, J. Panetier, J.W. Jurss

1:50 ENFL 173. Copper electrocatalysts with sub-surface oxygen for CO_2 reduction: An electronic-structure perspective. **S. Hedstrom**, C. Liu, A.R. Nilsson, L.G. Pettersson

2:10 ENFL 174. Withdrawn

2:30 ENFL 175. Superoxide-derived selective reduction of CO_2 to CO at low overpotentials in ionic liquid. Z. Wang, **Z. Huang**, A. Gupta, K.E. Riley, P. Kral

2:50 Intermission.

3:05 ENFL 176. Electrocatalytic reduction of CO_2: Routes toward efficient and selective copper-based electrocatalysts. **N. Kaneza**, S. Pan

3:25 ENFL 177. Engineered electrolyte-electrocatalyst nanocomposites for enhanced CO_2 electroreduction. **R.A. Elgammal**, T. Zawodzinski

3:45 ENFL 178. Electrochemical cycling strategy for selective and sustainable C_2H_2 production from CO_2 or CH_4 at atmospheric pressure using H_2O. **J.M. McEnaney**, B.A. Rohr, A. Nielander, A.R. Singh, J.K. Norskov, T.F. Jaramillo

4:05 ENFL 179. Surface engineering of earth-abundant transition metals by boron nitride for selective reduction of CO_2. **G. Hu**, Z. Wu, S. Dai, D. Jiang

4:25 ENFL 180. Direct conversion of CO_2 to surface-microporous graphene as efficient electrodes for supercapacitors. **Y.H. Hu**

4:50 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 237

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
F. Lin, K.A. See, *Organizers*
H. Chen, Y. Mo, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 181. Nucleation of dislocations and their dynamics in layered oxides cathode materials during battery charging. **A. Singer**

2:00 ENFL 182. Organic polymeric cathode materials for lithium-ion batteries. **B.P. Fors**

2:30 ENFL 183. Toward greener lithium-ion batteries: Aqueous binder-based $LiNi_{0.4}Co_{0.2}Mn_{0.4}O_2$ cathode material with superior electrochemical performance. **Z. Chen**, G. Kim, D. Chao, M. Copley, S. Passerini, Z. Shen

2:50 ENFL 184. Dynamics of surface metal–oxygen chemical environments in nickel-rich layered cathode materials. **J.D. Steiner**, J. Walsh, M. Rahman, B. Zydlewski, L. Mu, D. Nordlund, H. Xin, F. Lin

3:10 Intermission.

3:25 ENFL 185. Ions, electrons, and phonons: On the movement of charge through solids. **B.C. Melot**

3:55 ENFL 186. Closed loop recycling process for lithium ion batteries. **Y. Wang**

4:25 ENFL 187. Systematic evaluation of the stability and degree of dissociation of new sulfonimide salts. M. Huang, **S. Feng**, W. Zhang, L. Giordano, Y. Shao-Horn, J.A. Johnson

4:45 ENFL 188. Degradation-enabled protection of cathode materials for alkali metal ion batteries. **L. Mu**, F. Lin

5:05 ENFL 189. Designing high-performance battery materials using materials genomics screens. **B. Helms**, A. Ward, L. Li, T. Pascal, X. Qu, D. Prendergast, K. Persson

Section D
Ernest N. Morial Convention Center
Room 239

Road Map & Policy of Energy & Fuels

Climate Change & Energy

Cosponsored by ENFL
Q. Zhen, *Organizer*
S. Liu, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 190. Energy future. **A. Janetos**

2:15 ENFL 191. Extreme events and national climate assessments. **J. Lawrimore**, **D. Easterling**

3:00 Intermission.

3:10 ENFL 192. Global atmospheric composition, weather, and climate. **V. Ramaswamy**

3:55 ENFL 193. Climate change mitigation: Is it too late to recover? **F. Princiotta**

4:40 ENFL 194. Panel discussion on path forward related to the energy & environmental road map. **A. Pope**, **H. Jeffries**, **V.C. Garcia**, **D. Easterling**, **A. Janetos**, **V. Ramaswamy**, **F. Princiotta**, **B. Stewart**

Section E
Ernest N. Morial Convention Center
Room 240

Road Map & Policy of Energy & Fuels
Cosponsored by ENFL
Q. Zhen, *Organizer*
S. Liu, *Organizer, Presiding*

1:00 Panel Discussion.

1:00 ENFL 195. Road map and policy of

‡*Cooperative Cosponsorship*

energy: Panel Discussion about alternative energy. **M. Sanders**, **C. Sanders**

Section F
Ernest N. Morial Convention Center
Room 241

Hydrogen Energy: Production, Storage & Application

T. Autrey, V. Stavila, *Organizers*
F. Joo, K. Koh, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 196. Metal nanoparticle-catalyzed hydrogen generation from liquid-phase chemical hydrogen storage materials. **Q. Xu**

1:50 ENFL 197. Development of continuous high-pressure hydrogen evolution from formic acid in the presence of nano-Pd heterogeneous catalysts. **H. Kawanami**, H. Zhong, M. Iguchi, M. Chatterjee, Q. Xu

2:10 ENFL 198. Potentially viable CO_2 mediated H_2 storage materials for fuel cell applications. **C. Yoon**, H. Doh, S. Choi, H. Jeong, J. Kim

2:30 ENFL 199. Integrated CO_2 capture and conversion, a synergistic approach for liquid-based H_2 carriers. **D.J. Heldebrant**

2:50 ENFL 200. NH2-based heterogeneous cocatalyst boosts H2-production from HCOOH by the RuIII /P(CH2CH2PPh2)3 catalyst. M. Solakidou, Y. Deligiannakis, **M. Louloudi**

3:10 Intermission.

3:25 ENFL 201. Withdrawn

3:45 ENFL 202. Hydrogen production by dehydrogenation of formic acid using iridium catalysts. **Y. Himeda**, R. Kanega, L. Wang, N. Onishi, M. Ertem, J.T. Muckerman, E. Fujita

4:05 ENFL 203. Formulating thermodynamics for chemical compression in liquid carriers. K. Müller, K. Brooks, **T. Autrey**

4:25 ENFL 204. Withdrawn

4:45 ENFL 205. Role of solvent adducts in hydrogen dynamics of metal borohydrides: Neutron-scattering characterization. **M. Dimitrievska**, M. Chong, M. Bowden, W. Zhou, T. Autrey, T.J. Udovic

5:05 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 238

Shale Gas Extraction, Conversion & Utilization

L. Neal, T. Wang, *Organizers*
L. Fan, F. Li, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 206. Direct non-oxidative conversion of shale gas to chemicals: Catalyst selective activation, regeneration, and process intensification. **J. Hu**

2:10 ENFL 207. Mixed-oxide redox catalysts for light paraffin conversions under cyclic redox schemes. **F. Li**

2:45 ENFL 208. Aliovalent dopant-induced reactivity and recyclability enhancement in iron based oxygen carrier for chemical looping applications. **L. Qin**, **Z. Cheng**, M. Guo, Y. Liu, J. Fan, L. Fan

3:10 Intermission.

3:25 ENFL 209. Materials for chemical-looping with oxygen uncoupling (CLOU) for gas, liquid and solid fuels: Status of development. **T. Mattisson**, C. Linderholm, A. Lyngfelt

4:15 ENFL 210. Manganese-containing redox catalysts for selective hydrogen combustion under a cyclic redox scheme. **R.B. Dudek**, Y. Gao, J. Zhang, F. Li

4:40 ENFL 211. Molecular dynamics simulation and experimental study on nano-particles modified viscoelastic fracturing fluids. Z. Luo, **T. Wang**

5:05 ENFL 212. Extraction and storage of shale gas utilizing porous nanomaterials. **P. Villarreal**, I. Villavicencio, **S. Liu**, J. Liu

Nexus of Food, Energy, & Water: Adapting to Future Challenges
Sponsored by MPPG, Cosponsored by AGFD‡, ENFL‡ and ENVR‡

***Operando* Techniques for Catalytic & Photocatalytic Fuel Conversion Studies**
Sponsored by CATL, Cosponsored by ENFL

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Value Added from Agricultural Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

Magnetically Recoverable Catalysts
Sponsored by CATL, Cosponsored by COLL, ENFL and INOR

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
J.L. Liu, *Organizer*

8:00–10:00

ENFL 213. Conversion of sludge from waste water treatment plants via hydrothermal liquefaction. **M. Pimentel**, W. Jang, S. Kaiser, N. Humphries

ENFL 214. Stacked Pt-Ni/WC nanorod array electrocatalyst with gradient Pt-Ni alloy composition for ORR in PEM fuel cells. **F.M. Yurtsever**, M. Begum, M. Yurukcu, T. Karabacak

ENFL 215. Microwave characterisation techniques for hydrogen containing systems. **M. Barter**, **J. Hartley**, **M. Jones**, **A. Porch**

ENFL 216. Low-temperature hydrogen production from water and methanol using Pt/β-MoC catalysts. **L. Lin**, D. Ma

ENFL 217. Mesoporous MOFs for improved methane storage. **S. Banerjee**, Y. Fang, M.R. Bosch, E.A. Joseph, K. Ozdemir, H. Zhou

ENFL 218. Algal *oculata* biotemplated water-splitting nanocatalysts nickel/iron oxides. **M. Avram**, S. Elsaidi, T. Maxwell, B. Belingon, C. Li, W. Zhao

ENFL 219. Interaction between Mg_2FeH_6 and $LiNH_2$ for hydrogen storage. **W. Zhang**, H. Wang, T. He, J. Guo, G. Wu, P. Chen

ENFL 220. Graphene oxide films functionalized with perylenediimide-silane via a modified Langmuir-Blodgett technique. H.P. Rathnayake, **J.J. White**, J. Swain

ENFL 221. Distribution of products from Kraft lignin ablation with IR CO_2 laser. **D.J. Daniel**, M. Barekati-Goudarzi, D. Boldor, L. Khachatryan

ENFL 222. Study of Ni phases in spent fluid catalytic cracking (FCC) catalysts. **K. Triantafyllidis**, P.N. Trikalitis, V. Komvokis

ENFL 223. [Fe-Fe]-hydrogenase mimetic metallopolymers: Water solubility, enhanced rates, and aerobic stability in hydrogen evolution catalysts via polymer support. **W. Brezinski**, M. Karayilan, K. Clary, K. Matyjaszewski, D.H. Evans, D.L. Lichtenberger, R.S. Glass, J. Pyun

ENFL 224. Improving the performance of a hybrid model vehicle and reversible fuel cell with doped transition metal oxide nanocatalysts. P. Villarreal, I. Villavicencio, **S. Liu**, J. Liu

ENFL 225. Preparation of carbon nanodots from carrageenan and its application as sensitizer for nanostructured solar cells. **J.O. Bantang**, **D. Camacho**, **K.S. Schanze**

ENFL 226. Synthesis and characterizations of $B_3H_8^-$, $B_{10}H_{10}^{2-}$ and $B_{12}H_{12}^{2-}$ in various environments in the context of hydrogen storage and battery applications. **H. Hagemann**

Section C
Ernest N. Morial Convention Center
Room 239

Road Map & Policy of Energy & Fuels

Air Pollution, Human Health & the Environment

Cosponsored by ENFL
Q. Zhen, *Organizer*
S. Liu, *Organizer, Presiding*
V.C. Garcia, *Presiding*

7:00 Introductory Remarks.

7:05 ENFL 227. Understanding the linkage between air quality and human health. **A. Pope**

7:50 ENFL 228. Atmospheric chemical mechanisms and ozone reactivity scales. **H. Jeffries**

8:35 ENFL 229. Satellite measurements of chemical, meteorological, and climate variables. **B. Stewart**

9:20 ENFL 230. Accountability: Evaluating the impact of regulatory policies on air quality, human health, and the environment. **V.C. Garcia**

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 231

Issues & Challenges Related to Heavy, Light & Shale Oil Production & Processing

P. Rahimi, Y. Zhang, *Organizers*
J.J. Adams, C.F. Ovalles, *Organizers, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 231. Adhesion and surface energy of shale rocks. **D. Nguyen**, T. Phan, T. Hsu, J. Phan

8:25 ENFL 232. Kinetic precipitation of asphaltenes with the presence of inorganic solids. **M. Hoepfner**, W. Chaisoontornyotin, J. Zhang, S. Ng

8:50 ENFL 233. From design-to-practice: Low-viscosity acid platform to address carbonate stimulation needs. **A.J. Cairns**, M. Sayed, A. Gomaa, B.S. Aldakkan, K.R. Noaimi, R. Saini

9:15 ENFL 234. Stimulation of sandstone reservoirs: Oxidative triggered *in-situ* acid generation using ammonium-based salts. **A.J. Cairns**, K.L. Hull, M. Sayed, S. Metouri

9:40 Intermission.

9:55 ENFL 235. Self-healing polymer-cement composites for subsurface applications and beyond. **C. Fernandez**, K. Rod, M. Nguyen, F. Liu, P. Koech, V. Glezakou, J. Chun, N. Huerta, B. Kutchko

10:20 ENFL 236. Novel electroless plated Ni-P-C_3N_4 nanocomposite coating with outstanding performance. **M.K. Hassan**, E.M. Fayyad, A.M. Abdullah, G. Jarjoura, A. Mohamed, Z. Farhat

10:45 ENFL 237. Remediation of oilfield asphaltenic deposits: Chemical product design technology and near-well-bore application. **C. Russell**, E. Pohl

11:10 ENFL 238. Characteristic of morphology and iron species mobility on Fe poisoned FCC catalyst particles. **Y. Zhu**, H. Wu, F. Ren

11:35 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 232

Carbon Dioxide Conversion & Artificial Photosynthesis

Photocatalytic Conversion

Cosponsored by CATL, COMP and GEOC
S. Kawi, H. Lin, C. Liu, *Organizers*
Y.H. Hu, *Organizer, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 239. Nature inspired functional materials for solar energy manipulation and conversion. **H. Zhou**, T. Fan, D. Zhang

‡*Cooperative Cosponsorship*

8:20 ENFL 240. CO2 activation on bismuth oxide nanocluster modified rutile and anatase TiO2. **M. Nolan**

8:40 ENFL 241. Effect of defects in metal cluster/metal oxide photocatalysts for CO_2 photoreduction. **J. Chen**, S. Iyemperumal, N.A. Deskins

9:00 ENFL 242. Photo- and electrochemical conversion of CO_2 into fuels by novel nanostructured catalysts. **Y. Li**, F. Pan, X. Feng

9:20 ENFL 243. Utilizing NAD+/NADH analogs for fuel forming photoreductions. **S. Ilic**, K. Glusac

9:40 ENFL 244. Development of solar fuels photoanodes through combinatorial integration of multifunctional Fe-Ce oxide coatings on BiVO4 as a function of coating composition, loading, and electrolyte. **J. Haber**, D. Guevarra, A. Shinde, L. Zhou, F. Toma, J. Gregoire

10:00 Intermission.

10:10 ENFL 245. Design of photo/electrocatalysts from metal-organic precursors. **R. Xu**

10:35 ENFL 246. Activating carbon dioxide on metal oxide (CrOx, CuOx, CeOx) nanocluster modified TiO2. **M. Nolan**, S. Rhatigan

10:55 ENFL 247. Design concepts for assembling semiconductor/nanocarbon photoelectrodes employed in solar fuel generation. E. Kecsenovity, B. Endrodi, **C. Janaky**

11:15 ENFL 248. Understanding the chemical and physical mechanisms active in elevated temperature photocatalytic synthesis of hydrocarbons. S. Poudyal, M. Parker, **S. Laursen**

11:35 ENFL 249. Controllable hierarchical assembly of hollow tubular g-C_3N_4 with radially oriented nanosheets by solvent-free vapor-solid deposition-transition strategy. **L. Luo**, K. Li, A. Zhang, C. Song, X. Guo

Section C
Ernest N. Morial Convention Center
Room 237

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
F. Lin, Y. Mo, *Organizers*
H. Chen, K.A. See, *Organizers, Presiding*

7:55 ENFL 250. Crystal/interface structure vs. properties of Li-ion batteries. **F. Pan**

8:25 ENFL 251. *In-situ* and *operando* approaches for mechanistic insight of energy storage systems. **E.S. Takeuchi**, A.C. Marschilok, K.J. Takeuchi

8:55 ENFL 252. Investigating lithium-ion solvation structure and solid electrolyte interphase using multiscale vibrational spectroscopic and imaging techniques. **J. Nanda**, G. Yang, D. Voylov, D. Hallinan, R.E. Ruther, A.P. Sokolov, R. Sacci, I. Ivanov, G.M. Veith

9:25 ENFL 253. Probing bulk materials properties and the electrode-electrolyte interface with novel solid state NMR methodology. **M. Leskes**

9:55 Intermission.

10:05 ENFL 254. Asymmetric phase progression as the origin of hystersis in conversion electrodes. **K.W. Chapman**, K.M. Wiaderek, P.J. Chupas, N. Pereria, G. Amatucci

10:35 ENFL 255. Simulation of lithium ion transport through the complex electrode/SEI/electrolyte interface. **Y. Qi**

11:05 ENFL 256. Visualizing electro/chemical reactions at the nanoscale by *in-situ* TEM. **H. Xin**, M. Ge, Y. Chu

11:35 ENFL 257. Physical vapor deposition of Fe-N-C catalysts for PGM-free fuel cell electrodes. **N. Leick**, S. Kabir, K. Neyerlin, T. Gennett

Section D
Ernest N. Morial Convention Center
Room 239

Road Map & Policy of Energy & Fuels

Food, Energy, Water Resources & Economy: Evidence for Biophysical & Social Constraints on Society

Cosponsored by ENFL
Q. Zhen, *Organizer*
S. Liu, *Organizer, Presiding*
K.W. King, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 258. Systems thinking on the modern economy: Size and structure. **C. King**

9:00 ENFL 259. Scaling laws of biological and physical systems to inform economic growth and dynamic. **C. King**

9:45 Intermission.

10:00 ENFL 260. Money exchange model and energy over time: A general outlook. **C. King**

10:45 ENFL 261. Tales from the past: How indicators of societal structure during the Mayan collapse can inform us today. **C. King**

11:30 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 240

ENFL Distinguished Researcher Award: Symposium in honor of Joe D. Allison

A.A. Park, M.A. Reynolds, *Organizers*
E.B. Fox, D.J. Heldebrant, *Organizers, Presiding*

8:25 Introductory Remarks.

8:30 ENFL 262. How can analytical techniques add value to shale gas & oil production? A review of current technologies. **M.A. Reynolds**

8:55 ENFL 263. How hydraulic fracturing policy has shaped the US and world energy landscape. **E.B. Fox**

9:20 ENFL 264. Influence of water on hydrocarbon conversion reactions in zeolites. A. Gumidyala, K. Teel, J.L. White, B. Wang, **S. Crossley**

9:45 ENFL 265. Enabling clean and efficient combustion with GTL fuels. **A.L. Boehman**

10:10 Intermission.

10:25 ENFL 266. Upgrade options for NGL's. **M. Sardashti**

10:50 ENFL 267. Meeting future refinery fuel demands with the fluidized catalytic cracking unit. **F. Closmann**

11:15 ENFL 268. Extending stability in partial oxidation and Fischer-Tropsch catalysts. **J.D. Allison**

12:05 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 241

Hydrogen Energy: Production, Storage & Application

T. Autrey, V. Stavila, *Organizers*
M. Nath, G. Severa, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 269. Structural and electronic properties of photoabsorbers for water splitting: First principles calculations. **G.A. Galli**

8:20 ENFL 270. Electron-coupled proton buffers for water splitting. **M. Symes**

8:40 ENFL 271. Solar hydrogen production by catalytic photoelectrochemical devices for water splitting. **T. Yamada**, K. Domen

9:00 ENFL 272. Integrating *ab-initio* simulations and experimental characterization methods: Towards accelerated materials development for hydrogen production technologies. **T. Ogitsu**, J. Varley, T.A. Pham, B. Wood, S. Ptasinska, X. Zhang, K. Horsley, A. DeAngelis, N. Gaillard

9:20 ENFL 273. Visible light driven water splitting over $CaTiO_3/Pr^{3+}$-Y_2SiO_5/RGO catalyst by upconversion visible light to UV light. **G. Lu**

9:40 Intermission.

9:55 ENFL 274. Borohydride-based solid-state electrolytes with liquid-like sodium and lithium conductivity at room temperature. **A. Remhof**, Y. Yan, R.S. Kühnel, L. Dûchene, D. Rentsch, E. Cuervo Reyes, Z. Lodziana, H. Hagemann, C. Battaglia

10:15 ENFL 275. Controlled hydrogen release from metastable hydrides. **J.A. Graetz**, J. Vajo

10:35 ENFL 276. Advanced modeling of thermodynamics in complex metal hydrides for hydrogen storage. **S. Kang**, S. Bonev, T. Ogitsu, T. Heo, K.G. Ray, B. Wood

10:55 ENFL 277. Computational studies of kinetic mechanisms governing hydrogen interactions with complex hydrides. **B. Wood**, K.G. Ray, T. Heo, S. Kang, J. Lee, A. Baker, A.J. Rowberg, T. Ogitsu, R. Shi, L. Klebanoff, V. Stavila, M. Allendorf

11:15 ENFL 278. Results from a multi-laboratory comparison of hydrogen volumetric capacity measurements. **K. Hurst**, T. Gennett, P. Parilla

Section G
Ernest N. Morial Convention Center
Room 238

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Javier Garcia Martinez

K. Li, J.L. Liu, A.A. Park, M.A. Reynolds, *Organizers*
V. Valtchev, *Presiding*

8:25 Introductory Remarks.

8:35 ENFL 279. Innovative mesopore technology leads to formation of Rive Technology Inc. **D. Aldous**

9:05 ENFL 280. Early history of Rive Technology: Lessons learned in commercializing new technology. **L. Evans**

9:35 ENFL 281. Development and application of FCC catalyst integrating innovative Rive's mesoporous Y zeolite. **S. Kundu**, W. Cheng

10:15 Intermission.

10:35 ENFL 282. Dual role of surfactants as structure-directing agents and mesoporogens in the preparation of zeolites. **J.D. Rimer**, A. Chawla, R. Li, J.C. Palmer, J. Garcia Martinez

11:15 ENFL 283. Identifying the champion zeolite crystals in a powdered catalyst batch. **M.B. Roeffaers**

11:55 Concluding Remarks.

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Sponsored by CATL, Cosponsored by COMP and ENFL

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Food, Water & Energy from Sustainable Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 231

Issues & Challenges Related to Heavy, Light & Shale Oil Production & Processing

J.J. Adams, C.F. Ovalles, P. Rahimi, Y. Zhang, *Organizers*
P. Rahimi, Y. Zhang, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 284. Superior properties of oil sands derived crudes in refinery operation. **P. Rahimi**

‡*Cooperative Cosponsorship*

1:55 ENFL 285. Extraction of chloride from crude oil. **K. Huang**

2:20 ENFL 286. Chloride analysis in petroleum crude samples part 1: Evaluation of different detections techniques. **M. Dutta**, A. Pathilparampil, D. Quon, J. Tan, L. Poirier, L. Berhane, J. Nelson, F.A. Lopez-Linares

2:45 ENFL 287. Chloride analysis in petroleum crude samples part 2: Sample homogeneity impact on the analysis. D. Quon, J. Tan, T. Wei, A. Pathilparampil, L. Poirier, L. Berhane, J. Nelson, **F.A. Lopez-Linares**

3:10 Intermission.

3:20 ENFL 288. Predicting reactivity of feedstocks to vacuum resid hydroprocessing using nitrogen characterization. **C.F. Ovalles**, E. Rogel, M.E. Moir, J. Lopez, M. Hurt

3:45 ENFL 289. Co-processing of biofuels and heavy oil derived from oil sands. **M. Feng**

4:10 ENFL 290. Solvent extraction of spent hydrocracking catalyst. **C.F. Ovalles**, E. Rogel, M. Hurt, H. Morazan, K. Hench, M.E. Moir, V. Duma

4:35 ENFL 291. Accelerated aging test for fixed bed residue desulfurization catalyst. **W. Weiss**, P. Chatron-Michaud, B. Guichard

5:00 ENFL 292. Soft x-ray and TEM characterization of sulfur poisoned Pt/KL catalysts for the aromatization of hexane. **G. Jacobs**, W.D. Shafer, U. Graham, M. Martinelli, Y. Hu, B.H. Davis

Section B
Ernest N. Morial Convention Center
Room 232

Carbon Dioxide Conversion & Artificial Photosynthesis

Electro-Photo Catalytical Conversion

Cosponsored by CATL, COMP and GEOC
Y.H. Hu, S. Kawi, C. Liu, *Organizers*
H. Lin, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 293. Direct conversion of CO_2 into value-added C_{2+} hydrocarbons with high selectivity. **P. Gao**, S. Dang, X. Cui, H. Wang, L. Zhong, W. Wei, Y. Sun

1:50 ENFL 294. Hydrocarbons synthesis from CO_2 hydrogenation over Fe-based catalysts: Reaction pathways and kinetics from DFT. **X. Nie**

2:15 ENFL 295. Conversion of CO_2 into light olefins over iron supported on niobium oxide catalysts. **C.J. Mota**, I. da Silva

2:35 ENFL 296. Effect of alkali metals on CO_2 hydrogenation to hydrocarbons over zirconia supported CoCu bimetallic catalysts. **A. Hengne**, D. Yuan, L. Gevers, K. Huang

2:55 ENFL 297. Strategies of the anti-sintering catalysts design for the CO_2 hydrogenation to hydrocarbons. **w. li**, X. guo, C. Song

3:15 Intermission.

3:30 ENFL 298. Sophisticated structure control in catalyst design for CO2 conversion. **C. Xie**, C. Chen, D. Kim, G.A. Somorjai, P. Yang

3:50 ENFL 299. Direct transformation of carbon dioxide to value-added hydrocarbons by physical mixtures of Fe_5C_2 and potassium modified Al_2O_3. **J. L**, A. Zhang, M. Liu, C. Song, X. Guo

4:10 ENFL 300. Conversion of CO_2 into value-added chemicals over solid catalysts. **X. Guo**

4:35 ENFL 301. CO_2 hydrogenation over iron-based catalysts with various morphology and crystal face. **A. Zhang**, X. Guo, C. Song

5:00 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 237

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
F. Lin, K.A. See, *Organizers*
H. Chen, Y. Mo, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 302. Interfaces in Li-ion and Na-ion batteries – what more do we need to understand? **K. Edstrom**

2:00 ENFL 303. *In situ* TEM investigation of the electrochemical reaction pathways of sulfide materials with different alkali ions. **M.G. Boebinger**, M. Xu, D. Yeh, B.C. Miles, X. Ma, H. Chen, S. Hwang, D. Su, R. Unocic, M.T. McDowell

2:20 ENFL 304. Metal-free covalently-linked xanthenol dimers as model catalysts for OER: The O–O bond formation and their oxidative behavior. **M. Zoric**, K. Glusac

2:40 ENFL 305. Sodium layered oxide cathodes: Challenges and advances. **T. Rojo**, N. Drewett, N. Ortiz Vitoriano, E. Gonzalo, M. Galceran

3:10 Intermission.

3:25 ENFL 306. Liquid/solid state sodium based batteries for energy storage. **Y. Hu**

3:55 ENFL 307. High performance Li-doped cathode materials for Na-ion battery: Insights from electrochemistry, diffraction and NMR investigations. **L. Yang**, X. Li, X. Ma, S. Xiong, S. Zhao, P. Liu, Y. Tang, S. Cheng, Y. Hu, M. Liu, H. Chen

4:15 ENFL 308. Tetragonal Na_3SbS_4 electrolyte for all-solid-state sodium batteries operating below room temperature. **H. Wang**, Z. Hood, Y. Chen, J.K. Keum, A. Pandian, M. Chi, K. An, C. Liang, M. Sunkara

4:35 ENFL 309. Chalcogenide-based compounds as sodium superionic conductors. **S. Xiong**, Z. Liu, H. Rong, H. Chen

4:55 ENFL 310. Novel electrode materials for Li and Na ion batteries investigated by use of *ex-situ* and *in-situ* solid-state NMR spectroscopy. **P. Magusin**

5:15 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 239

Road Map & Policy of Energy & Fuels
Cosponsored by ENFL
Q. Zhen, *Organizer*
S. Liu, *Organizer, Presiding*
K.W. King, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 311. Principles of ecosystem resilience-based natural resource management in a changing world. **C. King**

2:15 ENFL 312. Perspectives on economics from oil and gas in tight sands and shale formations. **N.P. Schaffer**

3:00 Panel Discussion.

Section E
Ernest N. Morial Convention Center
Room 240

ENFL Distinguished Researcher Award: Symposium in honor of Joe D. Allison

E.B. Fox, D.J. Heldebrant, *Organizers*
A.A. Park, M.A. Reynolds, *Organizers, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 313. Alternative chemicals production from biomass via ionic liquids. **J. Chang**

1:55 ENFL 314. Tunable production of renewable fuels and chemicals via selective hydrodeoxygenation of hydropyrolysis vapors. **L. Zhang**, J. Lai, L. Nyadong, K. Gong

2:20 ENFL 315. Converting CO_2 to fuels and chemicals using new bimetallic catalysts. **C. Song**

2:45 ENFL 316. Photocatalytic conversion of natural gas. **Y.H. Hu**

3:10 Intermission.

3:25 ENFL 317. Nanostructure of a high-permeability, hydrogen-selective inorganic membrane. **S.T. Oyama**

3:50 ENFL 318. Advanced design and manufacturing center. **A.M. Gaffney**

4:15 ENFL 319. From electrons to economics: Designing an efficient water-lean CO_2 capture solvent system from atoms to ASPEN Plus. **D.J. Heldebrant**, P. Koech, V. Glezakou, R. Rousseau, D. Malhotra, R. Zheng, G. Whyatt, C. Freeman, M. Bearden

4:40 ENFL 320. Nanoparticle organic hybrid materials (NOHMs) for innovative CO_2 capture and conversion. M. Gao, W. Yu, **A.A. Park**

5:05 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 241

Hydrogen Energy: Production, Storage & Application

T. Autrey, V. Stavila, *Organizers*
T. Ogitsu, G. Severa, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 321. Electrocatalysis without precious metals. **P. Zelenay**

1:50 ENFL 322. Withdrawn

2:10 ENFL 323. Addressing transport losses in low-Pt and Pt-free PEM fuel cell cathodes. **S. Litster**

2:30 ENFL 324. Withdrawn

2:50 ENFL 325. Water reduction at low overpotentials with cobalt pyridyl-NHC electrocatalysts. **L. Chen**, X. Su, J.W. Jurs

3:10 Intermission.

3:25 ENFL 326. Hydrogen production by solar thermochemical water splitting: Searching for optimal nonstoichiometric perovskite oxides. **A.H. McDaniel**, D. Barcellos, M. Sanders, J.D. Sugar, R. O'Hayre

3:45 ENFL 327. Improving photocatalyst performance using nanomaterials. **C. Yang**

4:05 ENFL 328. Role of the electron's spin in water splitting. **R. Naaman**

4:25 ENFL 329. Experimental validation of a model for cryogenic hydrogen jet dispersion. **E.S. Hecht**, B. Roy Chowdhury

4:45 ENFL 330. Designing smart materials for efficient energy conversion: The story of transition metal chalcogenides. **M. Nath**, J. Masud, A. Swesi, U. De Silva, B.G. Amin, S. Umapathi, W.P. Liyanage

5:05 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 238

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Javier Garcia Martinez

K. Li, J.L. Liu, A.A. Park, M.A. Reynolds, *Organizers*
J.D. Rimer, *Presiding*

1:55 Introductory Remarks.

2:00 ENFL 331. Synthesis of chiral molecular sieves: A 30 year journey. **M.E. Davis**

2:40 ENFL 332. Bead-milling and post-milling recrystallization: A new methodology for the production of nano-sized zeolite. **T. Wakihara**

3:20 Intermission.

3:35 ENFL 333. Designer zeolites: Smaller, more accessible, better and affordable. **J. Gilson**, S. Mintova, V. Valtchev

4:15 ENFL 334. Greener synthesis of mesoporous zeolites. **F. Xiao**

4:55 Concluding Remarks.

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

***Operando* Techniques for Catalytic & Photocatalytic Fuel Conversion Studies**
Sponsored by CATL, Cosponsored by ENFL

‡*Cooperative Cosponsorship*

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Biomaterials Processing

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

R&D in the Chemical Catalysis for Bioenergy Consortium
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center Hall D

Chemistry: The Heart of Food, Energy & Water

S.L. Guertin, Z. Perry, *Organizers*

6:00–8:00

ENFL 335. Synthesis of glycidol and glycerol carbonate from transesterification of DMC and glycerol over mixed oxide catalysts. **L. Yajin**, D. He

ENFL 336. Fabrication of nano-sized attapulgite-based aerogels as anode material for lithium ion batteries. **Y. Lan**, D. Chen

ENFL 337. Mussel-inspired fabrication of polydopamine-functionalized attapulgite nanofibers as eco-friendly adsorbents for uranium adsorption. **Y. Liao**

ENFL 338. Tunability in organic electronics: Determination of surfactant role in directed self-assembly. **M.D. Rollings**, C. Boyle, D. Venkataraman

ENFL 339. New perspective into the mechanism for the highly facile interconversion of $(H)_2$ and $(\beta^2\text{-}H_2)$ in an iridium system: through an $(\beta^1\text{-}H_2)$ interaction? **H.T. Sartain**, C.M. Jensen

ENFL 340. Role of solvent on selective dehydrogenation of magnesium borohydride at moderate conditions. **P.Q. Nguyen**, M. Chong, M. Bowden, S. Shrestha, J. Yang, T. Gennett, T. Autrey, C.M. Jensen

ENFL 341. Freestanding 3D hierarchical carbon electrode enabled by poly(iaminonaphthalene) for energy storage and oxygen reduction reaction. **C. Ortuno-Quintana**, M. Acerce, K. Ramirez, J. Lu

ENFL 342. Norbornadiene–quadricyclane systems for molecular solar thermal energy storage. **M. Quant**, K. Moth-Poulsen

ENFL 343. Spherical aggregation of microalgae with acceleration of cell growth and lipid accumulation by encapsulation in hydrogels. **T. Yoshitomi**, S. Kaminaga, K. Yoshimoto

ENFL 344. Flake-like nanostructured copper oxide for pseudocapacitive energy storage. **P. Marathey**, R.K. Pati, I. Mukhopadhyay, A. Ray

ENFL 345. Stabilizing lithium metal anodes by atomic layer deposition of metal oxide on carbon network. **F. Zhang**, F. Shen, X. Han

ENFL 346. Design and economic evaluation of the TSA process for CO_2 capture from flue gas. X. Zhang, **F. Xiao**, **X. Wang**, F. Wang, N. Zhao

ENFL 347. Directly synthesis of dimethyl carbonate from methanol and CO_2 over $Fe_xZr_{1-x}O_2$ catalysts. A. Li, **N. Zhao**, F. Xiao

ENFL 348. Soxhlet extraction for post-synthetic generation of mesoporosity in MOFs. **E.A. Joseph**, M.R. Bosch, S. Banerjee, Y. Fang, K. Ozdemir, H. Zhou

ENFL 349. Synthesis and catalytic performance of highly siliceous ZSM-22. P. Niu, H. Xi, L. Jia, B. Hou, **D. Li**

ENFL 350. Preparation of full-range simulated TATP and odors analog. **J. Han**, J. Liu, Z. Hu, X. Liu, X. Ten

ENFL 351. Synthesization and characterization of dimethyl carbonate induced by electrode activated carbon. **J. Liu**, **Y. Zhu**, **J. Qiu**, Y. Li, H. Zhong

ENFL 352. Alkylamine loaded porous polymer networks for carbon dioxide capture. **H. Drake**, E.A. Joseph, G.S. Day, H. Zhou

ENFL 353. Evaluation of ethanol production from renewable cellulosic resources using process simulation tools. **D. Petrides**, D. Carmichael, C.A. Siletti

ENFL 354. Large scale algal oil production for bio-fuel use: Techno-economic analysis and evaluation. **D. Petrides**, D. Carmichael, C.A. Siletti

ENFL 355. Candy cane-like semi-interpenetrating polymer networks for enhanced fast-charging power source of electronics. **T. Wang**, S.K. Smoukov, K.D. Fong

ENFL 356. Natural polymer for a low-cost aqueous sustainable flow battery. **A. Mukhopadhyay**, J. Hamel, H. Zhu

ENFL 357. Forming pure shaped ZSM-5 zeolite bodies by steam assisted method and its application in methanol to aromatics reaction. **K. Zhang**, P. Liu, N. Zhao

ENFL 358. Confining Ni nanoparticles in honeycomb-like silica for coking and sintering resistant of partial oxidation of methane. **P. Liu**, K. Zhang

ENFL 359. Ni-containing poly-ionic liquid immobilized on solid SiO_2 as catalyst for crude oil aquathermolysis. **X. Guo**, R. Zou, J. Xu, T. Li, L. Li

ENFL 360. Enhancing performances of solution-processed inverted ternary small-molecule organic solar cells: Manipulating the host-guest donors and acceptor interaction. **W. Tan**, X. Zhu, Y. Min

ENFL 361. Designing efficient catalysts for CO_2 reduction based on porphyrinic metal-organic frameworks. **P. Zhang**, S. Yuan, X. Feng, Y. Li, H. Zhou

ENFL 362. Celstir processing of metal organic frameworks for increased gas storage. **A. Kirchon**, G.S. Day

ENFL 363. Engineering large Stokes shift heptamethine cyanine dyes for transparent luminescent solar concentrators (LSCs). **J. Zhang**, C. Yang, W. Sheng, B.G. Levine, R.R. Lunt, B. Borhan

ENFL 364. Withdrawn

ENFL 365. Increasing efficiency of ethanol production from crude glycerol and *Enterobacter aerogenes*. **A.M. Mayes**, D.L. Dillon, D.R. Caprioglio

ENFL 366. $Ni_xWO_{2.72}$ nanorods as an efficient electrocatalyst for oxygen evolution reaction. **Z. Xi**, A. Mendoza-Garcia, S. Sun

ENFL 367. Development of flexible solid electrolytes composed of plastic crystals (III): Effect of lithium salt species on ionic conductivity. **H. Yamada**, Y. Miyachi, Y. Takeoka, M. Rikukawa, M. Fujita

ENFL 368. Synthesis of hexagram-like ZnO photocatalysts co-doped with Ho and Yb for upconversion enhancement of dye sensitized solar cell performance. **J. Wu**

ENFL 369. Ultra-high thermal effusivity materials for ambient thermal energy harvesting. A. Cottrill, A. Liu, Y. Kunai, **V. Koman**, A. Kaplan, P. Liu, M. Strano

ENFL 370. Bimetallic nanoparticle catalysts for ammonia borane and formic acid dehydrogenation. **M. Muzzio**, C. Yu, S. Sun

ENFL 371. Surface functionalization of graphite felt electrode by N and O atomic co-doping for vanadium redox flow battery. H. Lim, J. Kim, **D. Lee**

ENFL 372. Synthesis and characterization of biodiesel fuels via transesterification of triglycerides with furfuryl alcohol. **A.L. Raley**, R.J. Franks

ENFL 373. Desulfurization of fuels using solid super acids. **M. Hurlock**, Q. Zhang

ENFL 374. Schiff base promoted hydrogenation of CO_2 to formic acid over gold nanocatalyst: A DFT calculation. **X. Yang**, Y. Huang

ENFL 375. Sulfonated copolyimides containing trifluoromethyl and phosphine oxide moieties: Studies on proton exchange membrane properties. **A.K. Mandal**, S. Banerjee

ENFL 376. Semifluorinated Poly(ether imide)s with cardo moiety: Synthesis, characterization and gas permeation studies. **R. Chatterjee**, S. Banerjee

ENFL 377. Hierarchical ZSM-5 aggregates with a compact shell synthesized in extremely dense gels. **T. Ma**, L. Zhang, Y. Song, Y. Shang, Y. Zhai, Y. Gong

ENFL 378. Withdrawn

ENFL 379. Pyrolysis of hydrolytic lignin dispersed in gas phase under IR laser irradiation. **M. Barekati-Goudarzi**, L. Khachatryan, D. Boldor

ENFL 380. Anaerobic digestion of the liquid phase from hydrothermal carbonization of municipal solid waste for evaluating and enhancing the biochemical methane potential. **K.J. Adams**, S. Kumar, B. Stuart

ENFL 381. Biodiesel production by *Jatropha curcas*. **A.N. Gondal**

ENFL 382. Synthesis of biodiesel fuels via transesterification using acorn (*Quercus sp.*) kernel oil as an alternative triglyceride source. **D. Bague**, R.J. Franks

ENFL 383. Catalytic hydrothermal liquefaction of Chlorella into bio-oil. **N.T. Humphries**, **S. Kaiser**, W. Jang

ENFL 384. Determination of the most effective asphaltene inhibitor at affecting the flocculation onset point in a medium crude oil. **H. Siegal**, G.C. Klein

ENFL 385. Investigation of novel coatings for aluminum particles for composite dielectric materials. **C. Alvarez-Sanchez**, K. Cook-Chennault, U. Sundar

ENFL 386. PAN-lignin polymer blends as carbon fiber precursors for high performance supercapacitors. **R. Jayawickramage**, J.P. Ferraris

ENFL 387. Zinc oxide nanowires in the active layer of an organic/inorganic hybrid solar cell. **K. Davis**, H.P. Rathnayake

ENFL 388. Molecular-level compositional analysis of condensates and crude oils by GC×GC MS and FT-ICR MS. **T. Yen**, J. Liu, R.P. Rodgers

ENFL 389. Determination of specific methanogenic activity and degradation rate constant of biomass samples from biodigesters of rural farms in Costa Rica. W. Ramos, E. Sánchez, **V. Chaves-Villarreal**, S. Rojas, M.F. Chacón, F. Jimenez, D. Zambrano

ENFL 390. System allowing automated thermal conductivity mapping as a function of temperature and pressure for hydrogen storage materials. **R.T. Bell**, N. Leick, M. Olsen, T. Gennett, P. Parilla

ENFL 391. Identifying hydrogen adsorption sites using *in-situ* DRIFTS. **S. Shulda**, J. Blackburn, P. Parilla, T. Gennett

ENFL 392. Photocatalytic H_2 production via a homogeneous tungsten catalyst. **H.P. Shirley**

ENFL 393. Utilization of waste fat, oil and grease (FOG) for the improvement of fermentative hydrogen production. **S. Saha**, S. Chang, M. Kurade, S. Chang, B. Jeon

ENFL 394. Two Janus faces in electrocatalysis: Activity versus stability of transition metal based electrocatalysts. **S. Barwe**, C. Andronescu, J. Masa, E. Ventosa, W. Schuhmann

ENFL 395. Atomic layer deposition used to stabilize H_2 storage materials. **N. Leick**, M. Martinez, K. Gross, S. Christensen

ENFL 396. Electronic structure calculations of hydrogen storage in Li decorated MOF built with graphyne. **D. Thogluva**

ENFL 397. *Ab-initio* modeling and experimental demonstration of metal oxides for solar thermochemical water splitting. **S. Millican**, I. Androshchuk, A.W. Weimer, C. Musgrave

ENFL 398. Selenophene-substituted benzothiodiazole-based polymer solar cells with high performances without additive. F. He, **X. Zhong**, H. Chen

‡*Cooperative Cosponsorship*

ENFL 399. Synthesis and characterization of N, Nβ-*bis*(salicylidene) ethylenediamine Copper complex for dye sensitized solar cells. **H.F. Sobhi**, W. Ghann, J. Uddin

ENFL 400. Quantum simulation for charge distribution in graphenes. Z. Liang, **P. Villarreal**, J.L. Liu, F. Tang

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 231

Bioenergy & Bio-Based Chemicals
Cosponsored by CELL
J. Fu, T. Morgan, *Organizers*
J. Chang, S. Fu, *Organizers, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 401. Soda green liquor combined with organosolv pretreatment to enhance enzymatic hydrolysis of sugarcane bagasse. **Y. You**, **J. Jiang**

8:50 ENFL 402. Fast hydropyrolysis of beetle killed lodge pole pine decorated with palladium nanoparticles. **H. Wise**, J. Gu, F.L. Resende, A. Dichiara

9:15 ENFL 403. STRONG® ebullated bed technology. **J. Liu**, X. Fang

9:40 ENFL 404. Retrosynthetic analysis of bio-derived fuels, and the identification of commodity feedstocks critical to potential commercialization. **J. Page**, P. Koech, D. Malhotra, K.O. Albrecht, D. Gaspar, L. Whitmore, C.M. Hudson, A. George, C. Moore, R. Wu, L.A. Silks, A.D. Sutton, C. Bailey, A. Zargar, L. Katz

10:05 Intermission.

10:15 ENFL 405. Application progress of residue hydroprocessing. **W. Gang**, J. Liu, X. Fang

10:40 ENFL 406. Ni/biochar catalysts for steam reforming of toluene as the biomass tar model compound. Z. Zhang, **Z. Du**, W. Li

11:05 ENFL 407. Homogeneous gas-phase pyrolysis of hydrolytic lignin under IR CO_2 laser irradiation. **L. Khachatryan**, M. Barekati-Goudarzi, D. Boldor

11:30 ENFL 408. Conversion of glucose to 5-hydroxymethylfurfural over zirconium phosphate catalyst. Y. Guo, **H. Zhao**

Section B
Ernest N. Morial Convention Center
Room 232

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in honor of Oliver C. Mullins

A.A. Park, A.E. Pomerantz, C. Reddy, M.A. Reynolds, *Organizers*
C. Reddy, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 409. Molecular structure of the heavy ends of petroleum and their evolution during petroleum generation. **A.E. Pomerantz**

8:35 ENFL 410. Studies on asphaltenes behavior at oil-water interfaces. **F. Liu**, S. Darjani, V. Pauchard, S. Banerjee

9:10 ENFL 411. Recent advances in mass spectrometric characterization of asphaltenes and crude oil. **H.I. Kenttamaa**

9:45 Intermission.

10:00 ENFL 412. Biodegradation of extended hopanes to 25-norhopanes in petroleum reservoirs: Insights from molecular mechanics. **K.E. Peters**

10:35 ENFL 413. Overview of heteroatom chemistry in fossil fuels. **S. Mitra-Kirtley**

11:10 ENFL 414. Upgrading asphaltenes by oil droplets striking a charged TiO_2-immobilized paper surface. Y. Lai, Z. Zhou, C. Basheer, **R.N. Zare**

11:45 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 237

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
F. Lin, Y. Mo, *Organizers*
H. Chen, K.A. See, *Organizers, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 415. Rechargeable magnesium battery systems: Electrolytes from simple Mg salts and sulfur-based cathodes. **J. Guo**

8:30 ENFL 416. Aqueous zinc ion battery with MoS_2 nanosheets cathode. W. Xu, X. Cheng, S.H. Rawal, Y. Xu, **Y. Wang**

8:50 ENFL 417. Can Mg^{2+} be intercalated into crystalline oxides? An update. **J. Cabana**

9:20 ENFL 418. Comparing morphology of magnesium and kinetics of its electrodeposition from varying classes of electrolytes. **B.M. Bartlett**

9:50 Intermission.

10:05 ENFL 419. Pathway to high energy density multivalent battery cathodes. **B.J. Ingram**, B. Key, J.T. Vaughey, J. Connell, P. Papa Lopes, T. Fister, S. Kim, P. Canepa, G.S. Gautam, g. Ceder, H. Yoo, R. Bayliss, J. Cabana

10:35 ENFL 420. Differences and similarities between Li, Na and Mg intercalation in transition metal oxides and sulfides. **A. Van der Ven**, M. Radin, J. Vinckeviciute, S. Kolli

11:05 ENFL 421. *In situ* electro-chemo-mechanics of electrode degradation in rechargeable batteries. **T. Zhu**

11:35 ENFL 422. Engineering MoS_2 for high-performance electrocatalytic hydrogen evolution. **G. Li**, L. Cao

Section D
Ernest N. Morial Convention Center
Room 239

Road Map & Policy of Energy & Fuels

M. King Hubbert: Is He Relevant?

Cosponsored by ENFL
S. Liu, Q. Zhen, *Organizers*
S. Bashir, C.A. Hall, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 423. Possible biophysical constraints on energy and hydrocarbon futures. **C.A. Hall**

8:40 ENFL 424. Historical usage of Hubbert analyses. **C.A. Hall**

9:10 ENFL 425. Hubbert analysis for the United States. **C.A. Hall**, **J.L. Hallock**

9:40 Intermission.

9:55 ENFL 426. Hubbert analyses for individual countries. **C.A. Hall**, **J.L. Hallock**

10:25 ENFL 427. Hubbert analysis for coal. **D. Rutledge**

10:55 ENFL 428. Historical perspective on development and application of energy return on investment (EROI). **C.A. Hall**

11:25 ENFL 429. Analysis of the energy return on investment (EROI) of existing fields. **M. Masnadi**, **A. Brandt**

Section E
Ernest N. Morial Convention Center
Room 240

X-Ray & Neutron Scattering in Energy Technologies

Diffraction

R.E. Winans, *Organizer*
K. Herwig, *Organizer, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 430. Magnesium and mobility: Utilizing X-rays and neutrons to investigate Mg mobility in spinel oxides. **S. Lapidus**, R. Bayliss, B. Key, G. Ceder, J.T. Vaughey, J. Cabana

8:30 ENFL 431. Neutron powder diffraction of energy storage materials. **A. Huq**

9:00 ENFL 432. Insights into high-pressure methane storage in metal-organic polyhedra via neutron powder diffraction. **E.D. Bloch**

9:30 ENFL 433. Shock induced carbon chemistry and fragment assembly revealed by static and time-resolved X-ray scattering. **M.A. Firestone**, B.S. Ringstrand, S. Seifert

10:00 Intermission.

10:10 ENFL 434. Neutron scattering studies of hydrogenous materials for next-generation energy storage. **M. Dimitrievska**, W. Tang, H. Wu, W. Zhou, T.J. Udovic

10:40 ENFL 435. *In-situ* neutron scattering studies of hydride conducting alkaline earth-metal hydrides. **G. Irvine**, J. Irvine, M. Jones

11:10 ENFL 436. Synthetic control and structural stabilization of Ni-rich layered oxides as high-energy cathodes for lithium-ion batteries. **J. Zhao**, L. Gao, W. Zhu

11:40 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 241

Hydrogen Energy: Production, Storage & Application

T. Autrey, V. Stavila, *Organizers*
D. Chandra, S. Kang, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 437. Developing ammonia as an energy vector–optimising sub-stoichiometric amide-based cracking catalyst performance. **W.I. David**, J. Makepeace, T. Wood

8:20 ENFL 438. Highly purified hydrogen production from ammonia for PEM fuel cells. **Y. Kojima**

8:40 ENFL 439. Bifrucation mechanisms in complex hydrides. Understanding formation of highly unstable intermediates formed in hydrogen release. I. Nayyar, **T. Autrey**

9:00 ENFL 440. Chemical design of competitive hydrogen storage characteristics in nanoscale metal hydrides. **J. Urban**

9:20 ENFL 441. Synergy of alkali amide/imide with transition metals in catalytic ammonia decomposition. **J. Guo**, L. Liu, P. Wang, F. Chang, X. Ju, G. Wu, P. Chen

9:40 Intermission.

9:55 ENFL 442. Highly efficient H_2 production by a 2 nanocatalyst engineered by flame spray pyrolysis (FSP). **Y. Deligiannakis**, V. Tsikourkitoudi, P. Stathi, E. Mouzourakis, M. Louloudi

10:15 ENFL 443. Sustainable photobiological hydrogen production via protein engineering of cyanobacterial hydrogenases. **A. Magnuson**, P. Raleiras, L.S. Mészáros, N. Khanna, H. Miranda, F. Ho, P. Lindblad, S. Styring

10:35 ENFL 444. Production of hydrogen from biomass via microbial electrolysis. **A. Borole**

10:55 ENFL 445. Hydrogen production based on biological water gas shift process. **H. Kim**, S. Kim

11:15 ENFL 446. Amorphous alloy membranes for hydrogen separation from CO_2 and other gases. S. Sarker, **D. Chandra**, B. Ruta, F. zontone, Q. An, T. Udovic, D. Isheim, D. Seidman, M. Dolan, D. Viano, G.M. King, J.R. Wermer

11:35 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 238

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Javier Garcia Martinez

K. Li, J.L. Liu, A.A. Park, M.A. Reynolds, *Organizers*
J. Gilson, *Presiding*

8:25 Introductory Remarks.

8:35 ENFL 447. Zeolite catalysis in biomass conversion: Stability, accessibility and confinement effects. **B.F. Sels**

9:15 ENFL 448. Catalytic pyrolysis of lignin with micro/mesoporous zeolites for the production of green phenolics and aromatics. **K. Triantafyllidis**

9:55 Intermission.

10:15 ENFL 449. Epoxidation of

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biodiesel over hierarchical TS-1-based catalysts: Improvement of diffusion or accessibility? **R. Glaeser**

11:35 ENFL 450. Award Address
(Kathryn C. Hach Award for Entrepreneurial Success Sponsored by the Kathryn C. Hach Award Fund). Discovery and commercialization of new catalysts engineered at the nanoscale. **J. Garcia Martinez**

12:15 Concluding Remarks.

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Sponsored by CATL, Cosponsored by COMP and ENFL

R&D in the Chemical Catalysis for Bioenergy Consortium
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 231

Bioenergy & Bio-Based Chemicals
Cosponsored by CELL

J. Fu, T. Morgan, *Organizers*
J. Chang, S. Fu, *Organizers, Presiding*

12:55 Introductory Remarks.

1:00 ENFL 451. Enhanced power generation in microbial fuel cells using material binding peptides. **J. Jahnke**, D.A. Sarkes, J. Terrell, M. Benyamin, D. Mackie, J. Sumner, D.N. Stratis-Cullum

1:25 ENFL 452. Bioconversion of anaerobic fermentation liquid of municipal sludge into microbial lipids by *Cryptococcus curvatus* using different cultivation strategies. **T. Mu**, X. Huang, J. Liu

1:50 ENFL 453. Flow field investigation to enhance the bioenergy production of high solid anaerobic digestion by particle image velocimetry (PIV). **H. Yuying**, J. Wu, S. Poncin, Z. Cao, Z. Li, H. Li

2:15 ENFL 454. Integration of graphene hybrids and photoactive protein bacteriorhodopsin for advancement of carbon-based photovoltaics. **C.C. Villarreal**, D. Pham, D. Rangel, A.J. Martinez, S. Prasad, V. Renugopalakrishnan, A.K. Mulchandani

2:40 ENFL 455. Demonstration of fusel alcohols as a platform for a tunable suite of high performance biofuel compounds for advance combustion strategies. **E. Monroe**, F. Liu, M. Tran-Gyamfi, A. George, R.W. Davis

3:05 Intermission.

3:15 ENFL 456. Study on changes of mineral structure by Fe (III) reducing bacteria and its role in inhibiting of clay swelling in low permeability reservoirs. **K. Cui**

3:40 ENFL 457. Hydrogen transfer from methanol over Ni/CMK-3 catalysts: The effect of different promoters. **Y. Xu**, C. Wang

4:05 ENFL 458. Synthesis, characterization, and application of novel materials. **N. Siraj**, S. Macchi, T. Viswanathan

4:30 ENFL 459. Optimization of wet microalgal biocrude production under the synergistic microwave and ultrasound effect. **V. Gude**, E. Martinez-Guerra

Section B
Ernest N. Morial Convention Center
Room 232

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in honor of Oliver C. Mullins

A.A. Park, C. Reddy, M.A. Reynolds, *Organizers*
A.E. Pomerantz, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 460. Award Address
(George A. Olah Award in Hydrocarbon or Petroleum Chemistry Sponsored by the George A. Olah Award Endowment). Asphaltenes: Nanometers to 100 kilometers; Nanoseconds to 50 million years. **O.C. Mullins**

2:15 ENFL 461. Production of spillphatenes following the 2010 Deepwater Horizon disaster. **C. Reddy**, C.P. Ward

2:45 Discussion.

3:15 Intermission.

3:30 ENFL 462. Imaging single molecules by scanning probe microscopy: Perspectives and examples in heavy oil characterization. **B. Schuler**, S. Fatayer, G. Meyer, L. Gross, A.E. Pomerantz, K.D. Bake, O.C. Mullins, E. Rogel, M.E. Moir, C.F. Ovalles, Y. Zhang, M. Harper, D. Kushnerick, F.G. van den Berg, M. Witt, D. Pena

4:00 ENFL 463. Theoretical studies of asphaltenes: Aromatic core analyzed by molecular orbital calculations with optical spectroscopy, and interfacial science analyzed by mesoscale simulations. **Y. Ruiz-Morales**

4:30 ENFL 464. Speciation and chemical composition of petroleum crude oil by Fourier transform ion cyclotron resonance mass spectrometry. **A.G. Marshall**, Y. Corilo, C. Hendrickson, J. Putman, L. Krajewski, D. Smith, C. Wesibrod, R.P. Rodgers

5:00 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 237

Innovative Chemistry & Materials for Electrochemical Energy Storage
Cosponsored by CATL, INOR and PMSE
H. Chen, F. Lin, Y. Mo, *Organizers*
K.A. See, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 ENFL 465. Dendritic growth of Li metal through solid-state electrolytes: Critical challenges, potential solutions. **N.J. Dudney**, A.S. Westover, R.D. Schmidt, R. Sacci, A. Huq

2:00 ENFL 466. Lithium-doped metal-organic thin films for battery interlayers and solid state electrolytes. **M. Young**, J. Elam

2:20 ENFL 467. Insight into fast ion conductors from solid-state NMR/MRI. **Y. Hu**, P. Chien, J. Zheng, M. Tang, X. Feng, J. Rosenberg

2:50 ENFL 468. Ambiguous influence of soft lattices on ionic transport. **W. Zeier**

3:20 ENFL 469. Mobility and stability descriptors of lithium ion conductors based on lattice dynamics. **S. Muy**, J.C. Bachman, L. Giordano, D.L. Abernathy, D. Bansal, O. Delaire, R. Kanno, F. Maglia, S. Lupart, Y. Shao-Horn

3:40 Intermission.

3:55 ENFL 470. Development of all-solid-state rechargeable batteries using amorphous materials with good ductility. **A. Hayashi**, A. Sakuda, M. Tatsumisago

4:25 ENFL 471. Fabrication of ultrathin solid electrolyte membranes of lithium thiophosphate via tiled assembly of shape-controlled building blocks. **Z. Hood**

4:45 ENFL 472. Argyrodite superionic conductors synthesized by liquid-phase techniques for all-solid-state lithium batteries. **S. Yubuchi**, M. Uematsu, A. Sakuda, A. Hayashi, M. Tatsumisago

5:05 ENFL 473. All-solid-state lithium-ion electrochemical cells based on lithium halide electrolyte. **J. Swanson**, M. Dondelinger, A. Smirnova

Section D
Ernest N. Morial Convention Center
Room 239

Road Map & Policy of Energy & Fuels

Energy Return on Investment (EROI)

Cosponsored by ENFL
S. Liu, Q. Zhen, *Organizers*
S. Bashir, C.A. Hall, *Presiding*

12:55 Introductory Remarks.

1:00 ENFL 474. EROI of new technologies. **C.A. Hall**

1:25 ENFL 475. Energy return on investment: Problems and solutions. **C. King**

1:50 ENFL 476. Money return on investment. **A. Berman**

2:15 ENFL 477. EROIs of solar technologies. **C.A. Hall**

2:40 Intermission.

2:50 ENFL 478. Conventional economics vs. biophysical economics. **C.A. Hall**, **K. Klitgaard**

3:15 ENFL 479. Economic and implications of EROIs. **C.A. Hall**

3:40 ENFL 480. Energy and human well being. **J. Lambert**

4:05 ENFL 481. Energy and collapsing states. **N. Ahmed**

4:30 ENFL 482. Energy and future environmental costs in Louisiana and Texas. **J.W. Day**, **A. Wegmann**

Section E
Ernest N. Morial Convention Center
Room 240

X-Ray & Neutron Scattering in Energy Technologies

K. Herwig, R.E. Winans, *Organizers*
A. Huq, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 483. Heteropoly acid polymer electrolyte development via small angle x-ray scattering under fuel cell relevant conditions. **A. Motz**, J. Horan, M. Kuo, A.M. Herring

2:00 ENFL 484. Thermo-responsive templates for conjugate polymer self-assemblies using block copolymers in aqueous solution. **C. Do**, Y. Han, J.Y. Carrillo, Z. Zhang, Y. Li, K. Hong, B. Sumpter, M.P. Paranthaman, G. Smith

2:30 ENFL 485. *In-situ* X-ray scattering and neutron imaging of combustion and combustion generated materials. **F. Ossler**

2:55 ENFL 486. Detecting aging in organic solar cells: An *operando* study. **P. Mueller-Buschbaum**, C. Schaffer, C. Palumbiny, S. Roth

3:25 Intermission.

3:30 ENFL 487. Structural water engaged disordered vanadium oxide nanosheets for high capacity aqueous K-ion storage. D.S. Charles, K. Page, J. Neuefeind, **X. Teng**

4:30 ENFL 488. Theory, experiment and predictions: Transition metal carbides (MXenes) for electrochemical capacitors. **H. Wang**, M. Naguib, W. Sun, L. Vlcek, K. Page, P. Kent, D. Wesolowski, Y. Gogotsi

4:55 ENFL 489. Functional lyotropic liquid crystal self-assembly: A well-defined platform for nanoconfined water dynamics studies. G. Jackson, S. Kim, S. Mantha, S. Diallo, K. Herwig, A. Yethiraj, **M.K. Mahanthappa**

Section F
Ernest N. Morial Convention Center
Room 241

Hydrogen Energy: Production, Storage & Application

T. Autrey, V. Stavila, *Organizers*
M. Bowden, T. Heo, *Presiding*

1:25 Introductory Remarks.

1:30 ENFL 490. Photocatalytic watersplitting: What can we learn from theory. **M.A. Zwijnenburg**

1:50 ENFL 491. Hydrogen storage in metal-organic frameworks. **H. Furukawa**, M. Kapelewski, H.Z. Jiang, T. Runcevski, Y. Lin, B.R. Barnett, K. Hou, G. Thiele, J.R. Long

2:10 ENFL 492. Understanding gravimetric and volumetric hydrogen cryo-adsorption trade-off in metal-organic frameworks (MOFs) and its link to material properties. G. Anderson, B. Schweitzer, R. Anderson, O. Farha, **D. Gomez-Gualdron**

2:30 ENFL 493. Enhanced hydrogen production using a zeolitic imidazolate

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framework membrane reactor. S. Lee, J. Kim, **D. Lee**

2:50 ENFL 494. Investigation into cationic ammonia borane dehydrogenation pathways including quantum tunneling considerations. A.D. Keith, D. Bellshaw, R. Hernandez-Lamoneda, **M. Gutowski**

3:10 Intermission.

3:25 ENFL 495. Mesoscale modeling of metal hydrides for hydrogen storage. **T. Heo**, S. Kang, R. Shi, B. Wood

3:45 ENFL 496. Activated magnesium boride based materials for hydrogen storage. **G. Severa**, C.M. Jensen, C. Sugai, S. Kim, B. Wood, S. Kang

4:05 ENFL 497. Hydride@graphene composites for hydrogen storage with improved kinetics and cyclability. L. Chong, **D. Liu**

4:25 ENFL 498. Bulk metallic system modeling using metal hydride dimer and trimer nanoclusters. **J.A. Darsey**

4:45 ENFL 499. Atomically thin interfacial suboxide key to hydrogen storage performance enhancements of magnesium nanoparticles encapsulated in reduced graphene oxide. **L. Wan**, Y. Li, E. Cho, J. Forster, S. Jeong, H. Wang, J.J. Urban, J. Guo, D. Prendergast

5:05 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 238

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Javier Garcia Martinez

K. Li, J.L. Liu, A.A. Park, M.A. Reynolds, *Organizers*
B.F. Sels, *Presiding*

1:25 Introductory Remarks.

1:35 ENFL 500. Properties and applications of metal oxide mesophases assembled from sustainable amine surfactants. C. Canlas, **T.J. Pinnavaia**

2:25 ENFL 501. Improving stability of zeolites and mesoporous materials in hot liquid water by hydrophobization with organosilanes. **D.E. Resasco**, T. Bui, D.T. Ngo

3:15 Intermission.

3:35 ENFL 502. Tuning zeolite accessibility by in-situ and post-synthesis methods. **V. Valtchev**

4:25 ENFL 503. Automated electron diffraction techniques for phase analysis and structure characterization of zeolite materials. **X. Zou**

5:15 Concluding Remarks.

Unconventional Catalysis Targeting Stable Molecules
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Towards Comprehension of Scale-Up & Multiscale Modeling of Catalysts
Sponsored by CATL, Cosponsored by COMP and ENFL

R&D in the Chemical Catalysis for Bioenergy Consortium
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

WEDNESDAY EVENING

Section A
Ernest N. Morial Convention Center
Room 231

Road Map & Policy of Energy & Fuels

Policy

Cosponsored by ENFL
S. Liu, Q. Zhen, *Organizers*
S. Bashir, C.A. Hall, *Presiding*

4:55 Introductory Remarks.

5:00 ENFL 504. Coal vs. gas: Are we condemning our grandchildren to feedstock poverty? **C.A. Hall**

5:30 ENFL 505. Energy trends in agriculture. **J. Schramski**

6:00 ENFL 506. Should we be burning coal, gas or developing PV? **S. Liu**

6:30 ENFL 507. Implications for chemistry futures: Panel Discussion. **C.A. Hall**

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 231

Alternative & Traditional Energy Resources & Energy Efficiency

Alternative Energy

A. Co, J.L. Liu, *Organizers*
Q. Zhang, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 508. Adsorptive desulfurization of heavy fuels using metal–organic frameworks. **Q. Zhang**

8:35 ENFL 509. Self-powered motion sensor using flow-less CNT sheet nanogenerator. **H. Song**, Y. Kim

9:00 ENFL 510. Fundamental insights into chemical looping combustion (CLC): A materials characterization approach to understanding mechanisms and size effects in oxygen carrier performance. **H. Alalwan**, S.E. Mason, D.M. Cwiertny, V.H. Grassian

9:20 ENFL 511. Structural correlations and transport mechanism of hydroxide in hydrated anion exchange membrane: A molecular dynamics simulation study. **D. Dong**, W. Zhang, A.C. Van Duin, D. Bedrov

9:40 Intermission.

9:55 ENFL 512. Effect of synthesis temperature on properties of ZSM-5/FDU-12 composite and its catalytic performance for the hydrodesulfurization of FCC diesel. **J. Fan**, Z. Zhao, P. Zheng, X. Wang, **A. Duan**, C. Xu, G. Jiang, J. Li

10:20 ENFL 513. Two new strategies to improve hypergolic ionic liquids as propellant fuels. **C. Sun**, **S. Tang**, X. Zhang

10:45 ENFL 514. Conservation of nitrogen in military propellant for ethanol production by algae. **P. Sanchez**, E. Cooke, P. Sheehan, K. Singer, W. Porubsky, D. Vail

11:05 ENFL 515. Novel pyrimidine-pyrene semiconductors for blue organic light-emitting devices. **J. Mathaga**, R.L. Perez, S. Ravula, I.M. Warner

11:25 ENFL 516. Low-cost and high-efficiency hierarchical catalyst for cyclic carbonate synthesis from CO_2. Y. Jian, **J. Meng**

11:50 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 232

Alternative & Traditional Energy Resources & Energy Efficiency

A. Co, J.L. Liu, *Organizers*
M. Smith, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 517. Microwave-assisted processes for chemical and fuel conversion. **M. Smith**, D. Shekhawat, V. Abdel-Sayed, C. Wildfire, M. Spencer, A.E. Stiegman

8:35 ENFL 518. Pumpless transport for passive aerospace fuel management solutions. **J. Mates**, R. Campos, J. Morrissette, A. Ghosh, C. Megaridis

9:05 ENFL 519. Study on liquid explosive simulant. **J. Liu**, D. Wang, X. Liu, Z. Hu, X. Ten

9:30 ENFL 520. Thermochemical gasification of biomass using the biomass-to syngas chemical looping process. **A. Tong**, D. Xu, Y. Zhang, Z. Cheng, L. Qin, T. Hsieh, M. Guo, C. Wang, E. Falascino, L. Fan

9:55 Intermission.

10:10 ENFL 521. Fabrication of fluorescent-superhydrophobic bifunctional coatings based-on reconstructed hierarchical structure with nanocellulose. **S. Fu**, C. Yu

10:40 ENFL 522. Further approach to kinetics study by combining TGA with *in-situ* FTIR. **J. Xiang**, Y. Cao

11:00 ENFL 523. Asphaltenes transport into hydrotreatment catalysts at high temperature. **J. Barbier**, F. Gaulier, B. Guichard, P. Levitz, D. Espinat

11:20 ENFL 524. Using electrospray ionization mass spectrometry as an ion chromatography confirmation tool for the determination of alkylamines and alkanolamines in scrubbing solutions. **T. Christison**, J. Rohrer

Section C
Ernest N. Morial Convention Center
Room 237

Alternative & Traditional Energy Resources & Energy Efficiency

A. Co, J.L. Liu, *Organizers*
A. Verma, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 525. Effects of surface ligands on the optoelectronic properties of the silicon nanowire. S. Alfalah, M. Shibl, **A. Verma**, R. Nekovei, M.M. Khader, M. Anantram

8:30 ENFL 526. Wastewater and energy nexus – evaluation of resource recovery potential through quantitative mass balance models. **V. Gude**, G. Sarpong

8:55 ENFL 527. Catalytic activities of transition metals in C-C bond cleavage and C-O bond coupling in ethanol oxidation reaction. B. Miao, Z. Wu, R. Wu, C. Zhong, **L. Wang**

9:20 ENFL 528. Featured microwave induced discharges for enhancing energy efficiency and promoting chemical reactions in a variety of fields. **J. Sun**

9:45 Intermission.

10:00 ENFL 529. Bimetallic Cu-Fe oxygen carriers for coal chemical-looping combustion. **P. Wang**, B. Howard, N. Means, D. Shekhawat

10:25 ENFL 530. Atmospheric oxidation and combustion of ketoalkoxy radicals. **M. Pan**, C. Protter, A. Davis

10:50 ENFL 531. Use of high temperature molten salts in advanced nuclear energy systems. **R.O. Scarlat**

11:15 ENFL 532. Ignition and combustion performances of high-energy-density jet fuels catalyzed by Pt and Pd nanoparticles. **X. E**, x. zhang, J. Zou

11:40 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 239

Electrochemistry in Fuel Cells & Flexible Fuels

V.I. Birss, V. Li, *Organizers*
J.L. Liu, R.A. Walker, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 533. Improving resilience and durability of SOFC anodes with secondary phases. **R.A. Walker**

8:30 ENFL 534. Dynamics of direct hydrocarbon PEM fuel cells. **E. Kong**, P. Ronney, S.S. Prakash

8:50 ENFL 535. Pyridine functionalized Pt/C: Ligand-mediated bifunctional catalyst for the enhanced oxygen reduction and methanol oxidation tolerance in fuel cells. **L. Lu**

9:10 ENFL 536. Electrochemically tuned cobalt hydroxide carbonate with abundant grain boundaries for highly

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efficient electro-oxidation of hydrazine. **X. Yan**, Y. Liu, J. Lan, Y. Yu, J. Murowchick, X. Yang, Z. Peng

9:30 ENFL 537. Electrocatalytic activities of ordered nanowire catalysts generated by self-assembled block copolymer templates. **L. Zhang**, C. Arges

9:55 Intermission.

10:10 ENFL 538. Self-supported hierarchical Ni_3S_2/Ni foam composite electrode with low onset potential and high durability for methanol oxidation. **G. Yuan**, Q. Wang, L. Wang, G. Liu, G. Li, L. Pan, J. Zou, X. Zhang

10:35 ENFL 539. Functional mesoporous carbon frameworks for efficient electrocatalytic oxygen and carbon dioxide reduction reaction. **F. Pan**, Y. Li

11:00 ENFL 540. Synthesizing intermetallic nanoparticle catalysts for fuel cell applications. Z. Qi, Y. Pei, **W. Huang**

11:25 ENFL 541. Improved oxygen reduction reaction using triple-component nanocatalysts. S. Wang, **V. Li**, Y. Wang, D. Qiao, C. Sun, **J.L. Liu**

11:50 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 240

Electrochemistry in Fuel Cells & Flexible Fuels

V.I. Birss, V. Li, *Organizers*
A. Reid, *Presiding*

7:55 Introductory Remarks.

8:00 ENFL 542. Physical approach for enhancing the electrocatalytic properties of nitrogen functionalized graphene nanosheets. **M. Jahan**, K. Li, G. Zhao

8:25 ENFL 543. Electrolytic combustion in the polyvinyl alcohol + hydroxyl ammonium nitrate solid propellant. **J. Lang**, J.K. Baird

8:50 ENFL 544. Facile synthesis of Pt-decorated mixed-phase CoCu bimetallic alloys supported on graphene oxide for applications in direct methanol fuel cells. **S.A. Alsaydeh**, A. Bin Yousaf, **S. Zaidi**, P. Kasak, M.K. Hassan

9:15 ENFL 545. Synthesis of ZIF-8 / functionalised acetylene black hybrid nanocomposites as non precious metal catalysts for ORR in fuel cells. **A. Singh**, R. Vedarajan, N. Matsumi

9:40 ENFL 546. TiO_2 nano tubes/ functionalised acetylene black composites decorated with pt nanoparticles as electrocatalyst for oxygen reduction reaction. **B. Santosh**, **R. Vedarajan**, **M. Noriyoshi**

10:05 Intermission.

10:15 ENFL 547. Clean fuel application using a tetranuclear cobalt(III) complex as a water oxidation catalyst. **A. Reid**, M.d. Hernandez, G. Kharel, R.K. Gurung, M.J. Celestine, A.A. Holder, D.A. Dixon

10:40 ENFL 548. Novel surface modification of carbon felt-supported Pd nanoparticles for ECH of oxygenates. **K. Koh**, A.J. Karkamkar, M. Derewinski

11:05 ENFL 549. Solid acid proton conductors: Insights into proton conduction mechanisms and advances in electrode architectures. **R.A. Elgammal**, T. Zawodzinski

11:30 ENFL 550. Energy-positive advanced wastewater treatment in anammox bioelectrochemical systems. **V. Gude**, U. Ghimire

Section F
Ernest N. Morial Convention Center
Room 241

X-Ray & Neutron Scattering in Energy Technologies

K. Herwig, *Organizer*
R.E. Winans, *Organizer, Presiding*

7:55 Introductory Remarks.

8:00 ENFL 551. New insights into dissociation behavior of methane and carbon dioxide hydrates at ambient pressure by *in situ* wide-angle x-ray scattering. **S. Lee**, S. Lee, A.K. Sum, R.E. Winans

8:30 ENFL 552. Withdrawn

9:00 ENFL 553. Probing the surface dissolution behavior of anorthite using *in-operando* X-ray reflectivity measurements for accelerated acid gas storage. M. Liu, **G. Gadikota**

9:30 ENFL 554. X-ray absorption spectroscopy and pair distribution function investigations of iodine-capture and deactivation of silver-exchanged mordenite for application in nuclear fuel reprocessing and advanced nuclear reactors. **C.W. Abney**, Y. Nan, L.L. Tavlarides

9:55 Intermission.

10:00 ENFL 555. Nafion interface structure, anisotropic ion transport, and re-entrant hydration vs. film thickness determined by *in-situ* neutron reflectometry. **J. Dura**, S. DeCaluwe

10:30 ENFL 556. Synchrotron X-ray study of metal nanoparticles synthesized via metal-in-Li solutions. **T. Xu**

11:00 ENFL 557. Bio-inspired single-atom cobalt catalysts with ehanced electrocatalytic performance. **T. Li**

11:30 ENFL 558. Thermally induced microstructural and structural changes in shales using multi-scale X-ray and neutron scattering measurements. **G. Gadikota**

Unconventional Catalysis Targeting Stable Molecules
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

THURSDAY AFTERNOON

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

ENVR

Division of Environmental Chemistry

S. Obare, *Program Chair*

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 346

Physics & Chemistry of Water Treatment: Symposium in honor of Professor Desmond F. Lawler

Membrane & Filtration Processes in Water Treatment

J. Darby, H. Garcia, J.A. Nason, *Organizers*
L.E. Katz, N.B. Saleh, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 1. Membrane-based processes at the water-energy nexus. **M. Elimelech**

8:45 ENVR 2. Point-of-use drinking water treatment with membrane filtration and desalination: A tale of two cities. **W. Walker**, I. Santiago

9:05 ENVR 3. Ion exchange membrane applications for nutrient separation in wastewater treatment. A. Alex, P. Yuan, V. Pavlovic, J. Barber, **Y. Kim**

9:25 ENVR 4. Trace organic rejection by reverse osmosis for potable reuse applications. **K. Howe**, D. Minakata, L.N. Breitner, M. Zhang

9:45 Intermission.

10:00 ENVR 5. Des Lawler: The early years. **P.C. Singer**

10:40 ENVR 6. Advancing filtration theory: Concurrent contributions of media surface roughness and ionic strength on particle deposition. **M. Emelko**, C. Jin, S. Normani

11:00 ENVR 7. Encountering the heterogeneous and evolving surfaces in the transport and transformation of aquatic nanoparticles. **B. Lau**

11:20 ENVR 8. Drinking water from the source to the tap: Ordering our priorities. **J.L. Schnoor**

Section B
Ernest N. Morial Convention Center
Room 347

Antibiotics & Antimicrobial Resistance: Developing Solutions to Address the Connectivity Between Air, Food, Water & Soil

Financially supported by AEESP
D.S. Aga, X. Li, A. Pruden, *Organizers*
P.J. Vikesland, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 ENVR 9. Metagenomic and ARG shifts during composting of antibiotic treated beef and dairy cattle manure. **I. Keenum**, R. Williams, E. Garner, P. Ray, K. Knowlton, A. Pruden

9:25 ENVR 10. Dissemination and propagation of ARGs mediated by conjugative multi-resistant plasmids. **Y. Luo**

9:45 ENVR 11. International comparison of the antibiotic "resistome" of raw sewage. **M.V. Prieto Riquelme**, J. Metch, E. Garner, A. Maile-Moskowitz, L. Angeles, D.S. Aga, I. Nambi, J. Larsson, H. Burgmann, T. Zhang, P.J. Vikesland, A. Pruden

10:05 Intermission.

10:20 ENVR 12. Differentiating ARG in non-viable sources towards improved understanding of hazard. **A. Eramo**, M. Yam, W. Morales Medina, N. Fahrenfeld

10:40 ENVR 13. Airborne bacteria and antibiotic resistance genes in $PM_{2.5}$ of Nanjing, China: Spatial-temporal variability and human inhalation risk. J. Xie, L. Jin, X. Luo, **X. Li**

11:00 ENVR 14. Dynamics of antibiotic resistance in sewers and sewer sediments. **A. Eramo**, S. Blanc, N. Fahrenfeld

11:20 ENVR 15. Spatial trends of antibiotics, metals, and antibiotic resistance genes in sediments. J.F. Kerrigan, K. Sandberg, D.R. Engstrom, T. LaPara, **W. Arnold**

11:40 ENVR 16. Environmental fate of antibiotics–impact of manure land application methods. **H.T. Le**, P. Ray, K. Knowlton, R.O. Maguire, K. Xia

Section C
Ernest N. Morial Convention Center
Room 348

Advances in the Transformations, Implications & Metrology of Carbonaceous Nanomaterials in the Environment

A.S. Adeleye, D. Goodwin, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 17. Photoenhanced oxidation of graphene oxide in the presence of free chlorine. **S. An**, J. Wu, J. Fortner

8:50 ENVR 18. (Photo)chlorination-induced transformation of graphene oxide: mechanism and environmental fate. **Y. Li**

9:15 ENVR 19. Colloidal stability and reduction of graphene oxide in marine waters. **A.S. Adeleye**, R.M. Burgess, K. Ho

9:40 ENVR 20. Nanoparticle interaction with isolated Gram-positive bacterial cell walls. **E.R. Caudill**, J. O'Rourke, K.P. Johnson, R. Tapia Hernandez, L. Zhu, A. Vartanian, C.J. Murphy, V. Feng, J.A. Pedersen

10:05 Intermission.

10:15 ENVR 21. Quantifying ROS reactivity of graphene oxide in aqueous media. **H. Hsieh**, **R.G. Zepp**

10:40 ENVR 22. Treatment of nitroaromatic explosives-contaminated water in aqueous phase by nano-sized carbon nanotube yarn. **S.R. Kanel**, I.E. Pavel Sizemore, D.M. Kempisty, M.N. Goltz

11:05 ENVR 23. Chemistry of Nano-CarboScavengers allows dual method rehabilitation of petroleum contaminated water. **S.K. Misra**, E. Daza, J. Scott, I.

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Tripathi, C.M. Promisel,, B. Sharma, J. Topczewski, S. Chaudhuri, D. Pan

11:30 ENVR 24. Silanization of nanocellulose and its influence on biodegradation and dispersion characteristics. **B. Frank**, D.P. Durkin, E.R. Caudill, D. White, M.L. Curry, J.A. Pedersen, H. Fairbrother

11:55 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 349

Chemistry of Drinking Water Distribution Systems & Infrastructure

D. Giammar, Y. Hu, H. Liu, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 25. Roles of corrosion inhibitors on simulated drinking water biofilm physical structures and responses to microplasma jet array treatment. P. Sun, G. Monroy, C. Huang, W. Chen, Y. Wang, Y. Wang, S. Boppart, **T.H. Nguyen**, J. Eden

8:50 ENVR 26. Heterogeneous lead phosphate nucleation at organic-water interfaces: Implications for lead immobilization. **Y. Hu**, C. Dai, J. Zhao, D. Giammar, J. Pasteris, X. Zuo

9:10 ENVR 27. Rates and pathways of controlling lead concentrations in lead pipes by orthophosphate addition. **Y. Bae**, L. Schattner, A. Ivarson, J. Pasteris, D. Giammar

9:30 ENVR 28. Effects of ortho- and polyphosphates on lead speciation in drinking water. **B. Trueman**, W. Krkosek, G.A. Gagnon

9:50 ENVR 29. Aggregation of lead phosphate nanoparticles: Implication for lead immobilization in pipe systems. **J. Zhao**, C. Dai, D. Giammar, J. Pasteris, Y. Hu

10:10 Intermission.

10:25 ENVR 30. Withdrawn

10:55 ENVR 31. Mineral characterizations of lead service line corrosion scale from Flint, Michigan. M. Wax, B. Ellis, **T.M. Olson**

11:15 ENVR 32. Lead levels in copper and lead service lines in Flint, Michigan. **S.J. Masten**, S. Davies, C.R. McPherson, S.W. Haider

11:35 ENVR 33. Geochemical drivers of lead exposure in Flint's drinking water distribution system. **S.P. McElmurry**, M. Dardona, M. Runho, J. Birbeck

Section E
Ernest N. Morial Convention Center
Room 350

Agro-Environmental & Energy Applications of Biochar/Hydrochar

Carbonization Processes & Modifications

N.D. Berge, C. Jeong, K. Ro, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 34. Selective extraction of value-added chemicals from hydrothermal carbonization bio-liquids. **S. Bae**, M. Choi, S. Lee, S. Park, Y. Hwang

8:30 ENVR 35. Sustainable water treatment materials via hydrothermal carbonization, secondary biofuel extraction, and activation of prickly pear cactus. L. Gao, M. Volpe, L. Fiori, **J.L. Goldfarb**

8:50 ENVR 36. Understanding the influence of feedstock properties and process conditions on products resulting from the hydrothermal carbonization of organics. L. Li, J. Flora, K. Ro, **N.D. Berge**

9:10 ENVR 37. Transformation of phosphorus during (hydro)thermal treatments of solid biowastes: Reaction mechanisms and implications for phosphorus reclamation and recycling. **R. Huang**, C. Fang, B. Zhang, Y. Tang

9:30 ENVR 38. Quantification of chemical states, dissociation constants, and oxygen functional groups on hydrochar. N. Saha, S. Mazumder, A. Saba, **M. Reza**

9:50 Intermission.

10:10 ENVR 39. Effects of ball milling on the physicochemical and adsorption properties of biochar. **B. Gao**, H. Lyu

10:30 ENVR 40. Production of magnetic hydrochars via hydrothermal carbonization (HTC) of metallic residues and wood. **B. Wirth**, M. Seiffert

10:50 ENVR 41. Turning un-hydrolyzed cellulosic lignin residue into surface-oxygenated biochar through hydrothermal carbonization and wet ozonization. O. Sacko, C. Li, G. Kharel, S. Abate, A. Sika, S. Kumar, **J.W. Lee**

11:10 ENVR 42. Ultrasound activation followed by amine functionalization: An efficient strategy for CO_2 capture by biochar. **R. Chatterjee**, B. Sajjadi, D.L. Mattern, W.W. Chen, N. Egiebor, Y. Liu

11:30 ENVR 43. Augmented photodegradation of methylene blue by titanium dioxide/biochar nanoparticles hybrid. **S. SafariMohsenabad**, K. von Gunten, M. Alam, M. Hubmann, D. Alessi

Section F
Ernest N. Morial Convention Center
Room 351

Aquatic Photochemistry

K.P. McNeill, *Organizer*
W. Arnold, S.G. Pati, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 44. Singlet oxygen quantum yields in different natural waters by various methods. **K.P. McNeill**

8:40 ENVR 45. Production of hydroxylating species from DOM model sensitizers. **K.D. Couch**, G. McKay, F.L. Rosario

9:00 ENVR 46. Kinetics studies and mechanistic considerations on the reactions of superoxide radical ions with dissolved organic matter. J. Ma, H. Zhou, S. Yan, **W. Song**

9:20 ENVR 47. $^1O_2$ phosphorescence as a probe for ^{3}DOMβ: Assessing triplet reactivity with sorbic acid. **K.J. Moor**, P.R. Erickson, K.P. McNeill

9:40 ENVR 48. Development of quantitative structure-activity relationships for triplet-sensitized aquatic photochemistry. **M. Taggart**, **S. Herring**, D.E. Latch, M. O'Connor, W. Arnold

10:00 Intermission.

10:10 ENVR 49. Effect of pH and wavelength on reactive oxidant production during chlorine photolysis. **C.K. Remucal**, D.M. Bulman

10:30 ENVR 50. Characterization of changes in dissolved organic matter properties and disinfection byproduct formation during solar photolysis of aqueous free chlorine. **T. Young**, W. Li, A. Guo, G. Korshin, S. Canonica, U. von Gunten, M.C. Dodd

10:50 ENVR 51. Critical analysis of reactive halogen species (RHS)-mediated photochemistry in halide-containing aquatic systems. **K. Parker**, A. Mishrra

11:10 ENVR 52. Sulfate radical oxidation of aromatic contaminants: A detailed assessment of density functional theory and high-level quantum chemical methods. **B.M. Wong**, S. Pari, H. Liu, I.A. Wang

11:30 ENVR 53. Mechanism of ferric oxalate photolysis from ultrafast infrared spectroscopy. **B. Gilbert**, D.M. Mangiante, R.D. Schaller, P. Zarzycki, J. Banfield

Section G
Ernest N. Morial Convention Center
Room 342

Novel Membrane-Based Technology for Water Purification & Desalination

New Membrane Materials

D. Jassby, B. Mi, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 54. Artificial water channels. **M. Barboiu**

8:30 ENVR 55. Novel graphene-based additive for membrane surface modification. **X. Zhu**, L. Zhang, B. Chen

8:50 ENVR 56. GO mediated surface modification of polyamide membrane with zwitterionic polymer brush and peptide to control the biofouling via "bacteria-defending and -attacking" strategies. **W. Ma**, S. Nanni, T. Chen, A. Tirafferri, M. Rahaman

9:10 ENVR 57. Electrospraying ultrathin reduced graphene oxide (rGO) membrane for water desalination. **Q. Huang**, S. Zheng, Z. Wang, L. Lin, X. Zhang, B. Mi

9:30 ENVR 58. Demonstration of *in situ* membrane surface cleaning and reformation with modification of crumpled graphene oxide – magnetite composites. **Q. Zeng**

9:50 Intermission.

10:00 ENVR 59. Applications of graphene oxide membranes. **R. Joshi** , B. Lian, Y. You, V. Sahajwalla, G. Leslie, V. Chen, H. Bustamante

10:30 ENVR 60. Development of graphene frameworks membranes for separation of immiscible liquids. **C.M. Mai Van**

10:50 ENVR 61. Heterostructure membranes made from stacked-two-dimensional nanomaterials: Tuning the interlayer-spacing for aqueous phase separation. **S. Zheng**, Q. Tu, B. Mi

11:10 ENVR 62. Two-dimensional metal carbides (MXenes): New frontiers for water treatment applications. **K.A. Mahmoud**, K. Rasool, R. Pandey

11:30 ENVR 63. Size-dependent antimicrobial activities of chemically exfoliated MoS_2 nanosheets coated membrane surfaces. **Y. Zhao**, X. Zhang, S. Hermanowicz, B. Mi

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Mechanisms & Selectivity

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LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

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Nanocellulose-Based Technologies

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Challenge & Opportunity in Lignin Valorization
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SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 346

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Physics & Chemistry of Water Treatment: Symposium in honor of Professor Desmond F. Lawler

Alternative Water Sources & Treatment Applications

L.E. Katz, J.A. Nason, N.B. Saleh, *Organizers*
J. Darby, H. Garcia, *Organizers, Presiding*

1:30 ENVR 64. Harvesting urban stormwater runoff for water supply. **R.G. Luthy**, S. Spahr, N. Ashoori, M. Teixido Planes, D.L. Sedlak

2:10 ENVR 65. From drinking water to stormwater: The role of a spore's electrical double layer in surface interactions. **A. Mikelonis**, S. Youn, K. Ratliff

2:30 ENVR 66. Accurate estimation of DBP precursors using short-term and thermally accelerated protocols. **D.A. Reckhow**, C. Dozier

2:50 ENVR 67. Sustaining water availability in rural communities: Expanding use of poor quality waters. **D.D. Reible**, C. Na

3:10 Intermission.

3:30 ENVR 68. Rainwater for drinking: Science, technology, practice and case studies. **M. Han**

4:10 ENVR 69. Potential for disinfecting rainwater with nanosilver-enabled ceramic filters. **M. Kirisits**, T. Kim, L.S. Rowles III, D.F. Lawler, N.B. Saleh

4:30 ENVR 70. Investigating key indicators impacting plate health, aluminum generation, and fluoride treatment in electrocoagulation defluoridation treatment systems. **K.A. Alfredo**, M. Jain, P. Nagarnaik, P. Labhasetwar

4:50 ENVR 71. Boron removal from hydraulic fracturing flowback water by chemical and electrocoagulation: Mechanisms and limitations. **S. Chellam**

5:10 ENVR 72. Application of physical/chemical treatment processes to agricultural waste: Recovering nutrient-laden particles from poultry litter. U. Shashvatt, C. Portner, S. Musa, H. Aris, **L.M. Blaney**

Section B
Ernest N. Morial Convention Center
Room 347

Antibiotics & Antimicrobial Resistance: Developing Solutions to Address the Connectivity Between Air, Food, Water & Soil

Impacts of Treatment

Financially supported by AEESP
D.S. Aga, A. Pruden, P.J. Vikesland, *Organizers*
X. Li, *Organizer, Presiding*

1:30 ENVR 73. Nucleic acid reactivity and functional fate in drinking water and wastewater treatment processes. **K. Wigginton**

2:00 ENVR 74. Development and application of predictive models for antibiotic resistance gene degradation and deactivation kinetics during bench-scale and full-scale disinfection processes. **H. He**, P. Zhou, K. Shimabuku, X. Fang, A. Anderson, M.C. Dodd

2:20 ENVR 75. Effects of metals on the relative abundance of antibiotic resistant bacteria in drinking water. **A. Kappell**, K. Harrison, P.J. McNamara

2:40 ENVR 76. Antibiotic resistance in anaerobic membrane bioreactors treating synthetic domestic wastewater and a blend of real domestic wastewater and manure. **E. Rice**

3:00 Intermission.

3:15 ENVR 77. Evaluation of integrated algae-wastewater treatment systems to remove antibiotics and reduce downstream antibiotic resistance. **K. Grimes**, L.M. Colosi

3:35 ENVR 78. Polyvalent bacteriophage therapy to suppress antibiotic-resistant bacteria in environmental systems. **P. Yu**, P.J. Alvarez

3:55 ENVR 79. Silver nanoparticles induce antibiotic resistance in *Pseudomonas aeruginosa*. **B.A. Chambers**, S.K. Smith, M.J. Kirisits

4:15 ENVR 80. Physiological response of *Shewanella oneidensis MR-1* to spatial gradients of ciprofloxacin concentration. **R.E. Alcalde**, L. Zhou, J. Deng, R. Sanford, B. Fouke, C.J. Werth

4:35 ENVR 81. Comparison of virus concentration methods from various water matrices for detecting the viral resistome. **K. Langenfeld**, R. Cable, M. Duhaime, K. Wigginton

4:55 ENVR 82. Role of motility in *Escherichia coli* response to antibiotic gradients in microfluidics. **L. Zhou**, J. Deng, Y. Dong, R.E. Alcalde, R. Sanford, B. Fouke, C.J. Werth

5:15 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 348

Advances in the Transformations, Implications & Metrology of Carbonaceous Nanomaterials in the Environment

A.S. Adeleye, D. Goodwin, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 83. Microbial transformation and plant uptake of multi-walled carbon nanotubes. **Y. Yang**, Y. You, K.K. Das, J. Chan, F. Barrios-Masias, P. Verburg, S. Poulson, X. Wang, B. Xing

2:05 ENVR 84. Quantification of multiwall carbon nanotubes in plant tissues using digestion-coupled programmed thermal analysis. **K.K. Das**, Y. Yang, B. Xing, X. Wang, J. Chow, L. Bancroft

2:30 ENVR 85. Single and combined effects of carbon nanotubes and surfactant on bioaccumulation and translocation of pyrene and 1-methylpyrene in maize seedlings: Multicompound exposure scenarios. **H. Zhang**, Y. Liu, X. Shen, M. Zhang, Y. Yang, S. Tao, X. Wang

2:55 ENVR 86. Microplastic exposure assessment from the perspective of nanoparticle research. **T. Hueffer**, A. Praetorius, S. Wagner, F. Von Der Kammer, T. Hofmann

3:20 Intermission.

3:30 ENVR 87. Assessment of graphene oxide/polymer nanocomposite degradation from different metrolology approaches. **D.G. Goodwin**, T. Lai, A. Campos, V. Reipa, J.M. Gorham, T. Nguyen, L. Sung

3:55 ENVR 88. Characterization of engineered nanomaterial release from nanoenabled products following accelerated and natural weathering. **R. Lankone**, J. Wang, K. Challis, Y. Bi, D. Hanigan, Y. Wang, M. Garland, R. Reed, T. Zaikova, P.K. Westerhoff, L.M. Gilbertson, J.F. Ranville, H. Fairbrother

4:20 ENVR 89. Degradation of solid state C_{60} fullerene by UV irradiation under environmentally relevant conditions. A. Carboni, R. Helmus, P. de Voogt, K. Kalbitz, **J. Parsons**

4:40 ENVR 90. Reactions of hematite in the presence of carbon nanoparticles. **A.M. Johansen**, H. Casique, A. Reddy, J. Rodriguez, J. Rodriguez, S. Bradford

5:00 ENVR 91. Surface oxidation and iron speciation on carbon nanoparticles for precise air pollution models. **A. Pattammattel**, V. Leppert, H.J. Forman, P.A. O'Day

5:20 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 349

Chemistry of Drinking Water Distribution Systems & Infrastructure

D. Giammar, Y. Hu, H. Liu, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 92. Crucial chemistry at water-arsenopyrite interfaces during managed aquifer recharge. **Y. Jun**, C. Neil, J. Yang, D. Schupp

2:05 ENVR 93. Multiscale modeling of dead-ends of drinking water distribution systems: Disinfectant transport to DBP formation to lead release. A.A. Abokifa, **P. Biswas**

2:35 ENVR 94. Factoring physics into local and global assessments of nitrogen pollution. **S. Grant**

3:05 ENVR 95. Recent developments for chromium(VI) removal from groundwaters. **I. Katsogiannis**, A. Zouboulis, M. Mitrakas

3:25 Intermission.

3:40 ENVR 96. Building plumbing safety: Right sizing tomorrow's water systems for efficiency, sustainability, and public health. **A.J. Whelton**, M. Salehi, J. Mitchell, J. Rose, A. Nejadhashemi, J. Beecher, E. Dreelin, A. Shah, T. Gim Aw, M. Syal

4:10 ENVR 97. Lead release resulting from galvanic corrosion in a three-metal system consisting of lead, copper and stainless steel in drinking water. J. Lin, D. Ng, **Y. Lin**

4:30 ENVR 98. Investigating the relationship between discolored water from galvanized iron corrosion and source water conditions. **M. Tang**, V. Nystrom, K. Pieper, J. Parks, M. Edwards

Section E
Ernest N. Morial Convention Center
Room 350

Agro-Environmental & Energy Applications of Biochar/Hydrochar

Agricultural & Energy Applications

N.D. Berge, C. Jeong, K. Ro, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 99. Matching hydrochar characteristics with application requirements to improve agricultural nutrient use efficiency. **J. Libra**, J. Kern

2:00 ENVR 100. Impact of biochar and biochar-compost mixture application on cotton yield and nutrient runoff losses in four consecutive planting seasons. **C. Jeong**, H. Ku, K.S. Ro

2:20 ENVR 101. Influence of biochar addition on the soil microbial community responses in poultry manure applied soybean crop systems. **J. Ham**, R. Calderon, C. Jeong, K. Ro

2:40 ENVR 102. Biochar application effects on water quality in two different textured soils. **N.D. Tafti**, J.J. Wang, J. Park, M. Wang

3:00 ENVR 103. Effect of biochar on soil water content, nutrient release, greenhouse gas and ammonia emissions, and crop growth. **S. Dodla**

3:20 Intermission.

3:40 ENVR 104. New perspectives for biochar utilization under food-water-energy nexus. **M. Urgun-Demirtas**

4:00 ENVR 105. Effects of manure-derived biochar on solid state anaerobic digestions of manure. **H. Jang**, Y. Choi, E. Kan

4:20 ENVR 106. Effects of feedstock, pyrolysis conditions, and activation on removal of odorous compounds. **K. Ro**, O. Hwang, S. Lee, D. Han, S. Cho, M. Spiehs, B. Woodbury

4:40 ENVR 107. Biochar surface oxygenation through ozonization for enhanced cation exchange capacity. M. Huff, S. Marshall, H. Saeed, **J.W. Lee**

5:00 ENVR 108. Hydrochar application to adsorption of contaminant and gas and energy storage. X. Zhu, **S. Zhang**, J. Chen

Section F
Ernest N. Morial Convention Center
Room 351

Aquatic Photochemistry

W. Arnold, *Organizer*
K.P. McNeill, S.G. Pati, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 109. Effects of ozone on the photophysical and photochemical properties of dissolved organic matter. **F. Leresche**, T. Kurtz, G. McKay, S. Canonica, U. von Gunten, F.L. Rosario

1:55 ENVR 110. Dissolved organic matter (DOM) characterization and enhanced photoreactivity in constructed wetlands for wastewater treatment. **A. Sardana**, B. Cottrell, T.N. Aziz

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2:15 ENVR 111. Impact of dissolved organic matter composition on the production of photochemically-produced reactive intermediates in the St. Louis River. **S. Berg**, K.H. Wammer, C.K. Remucal

2:35 ENVR 112. Impact of dissolved organic matter composition variability on indirect photolysis of contaminants in the St. Louis River. **K.H. Wammer**, Q.T. Whiting, J.A. Herrli, S. Berg, C.K. Remucal

2:55 ENVR 113. Critical evaluation of models for chromophoric dissolved organic matter optical properties and photochemistry. **G. McKay**, F.L. Rosario, J.A. Korak

3:15 Intermission.

3:25 ENVR 114. Photochemistry of natural organic matter (NOM) in natural waters: Implications to reactive oxygen species generation and redox cycling of iron. **S. Garg**, D. Waite

3:45 ENVR 115. Singlet oxygenation of Domoic acid: Mechanisms and biological significance. **M. Jaramillo**, K.E. O'Shea

4:05 ENVR 116. Our dusty future: Singlet oxygen production by illuminated road sediment and winter traction material. **S.A. Styler**, P.D. Milner, J.R. Kwasny, A. Duarte de Marins Costa:, L. Gan, S.R. Schneider

4:25 ENVR 117. Evaluating the magnitude of partial photo-oxidation of organic carbon in sunlit surface waters. **C.P. Ward**, C. Reddy, R.M. Cory

4:45 ENVR 118. Temperature dependence of the fluorescence of dissolved organic matter: Implications for DOM photophysics. **G. McKay**, J.A. Korak, F.L. Rosario

Section G
Ernest N. Morial Convention Center
Room 342

Novel Membrane-Based Technology for Water Purification & Desalination

Membrane Fouling & Surface Modification

D. Jassby, B. Mi, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 ENVR 119. Withdrawn.

2:00 ENVR 120. Optimizing layer by layer approach via ultrasonic spray technique: A case study of depositing anatase titanium dioxide and polydopamine to reduce fouling while enhancing water flux. **A.J. DeStefano**, D. Li

2:20 ENVR 121. Facile deposition of photo-mobile materials on polymeric membranes achieving self-cleaning properties. **H. Lin**, S. Ramanan, N. Shahkaramipour, T. Tran

2:40 ENVR 122. Mitigation of humic acid fouling on ultrafiltration membranes in a photocatalytic system. **R. Zhu**, A. Diaz, Y. Sun, S. Solares, D. Shuai

3:00 Intermission.

3:10 ENVR 123. Membrane treatment of oil and gas wastewater: 7 years of resaerch experience. **T.Y. Cath**

3:40 ENVR 124. Zwitterion-modified forward osmosis membrane used for shale oil produced water treatment. **R.R. Kommalapati**, **H. Du**, S. Potluri, V. Botlaguduru

4:00 ENVR 125. Comparison and characterization of biofilm removal by different chemical cleaning solutions for water treatment applications. **C. Kim**, S.L. Walker, D. Jassby

4:20 ENVR 126. Backwashing of hollow fiber membranes during constant flux microfiltration of secondary wastewater effluent: Modeling and mechanisms of physically irreversible fouling. **K. Gupta**, S. Chellam

4:40 ENVR 127. Tuning the microstructure of functional layer for improved wastewater treatment performance of polymeric composite membrane. **J. Meng**

5:00 ENVR 128. Probing nanoscale hydrophobicity and chemical distribution of surface modified polyethersulfone (PES) membranes. **W. Fu**, W. Zhang

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

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Challenge & Opportunity in Lignin Valorization
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MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 346

Physics & Chemistry of Water Treatment: Symposium in honor of Professor Desmond F. Lawler

Particles & Advanced Oxidation

H. Garcia, L.E. Katz, N.B. Saleh, *Organizers*
J. Darby, J.A. Nason, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 129. Withdrawn.

8:45 ENVR 130. Manganese and iron control: the critical role of particles and surfaces. **J.E. Tobiason**

9:05 ENVR 131. Overcoming barriers limiting widespread adoption of catalytic destruction of nitrate in drinking water. **C.J. Werth**, A. Bergquist, M. Bertoch, S. Seraj, P. Kunal, S.M. Humphrey

9:25 ENVR 132. Utilizing organophosphates to control particle properties: From antiscalants in desalination to iron-mediated persulfate oxidation. **L.F. Greenlee**

9:45 Intermission.

10:00 ENVR 133. Unexpected and potentially toxic products of advanced oxidation processes. **D.L. Sedlak**, C. Prasse, J. Van Buren

10:40 ENVR 134. Enzymatic treatment to remove pharmaceutical and personal care products (PPCPs) from municipal wastewater effluents. **K.A. Kinney**, H. Garcia, D.F. Lawler, C.P. Whitman, W.H. Johnson, O. Haugland

11:00 ENVR 135. Advancing catalysts and catalytic processes for treating oxyanion water pollutants – moving beyond palladium and developing hybrid reactor systems. **T.J. Strathmann**, X. Huo, J. Liu, Y. Wang

11:20 ENVR 136. Kinetic models for advanced oxidation-reduction processes. **B. Batchelor**

11:40 ENVR 137. Electron donating capacity as a novel tool to assess oxidation processes
. **U. von Gunten**, L. Oennby, K. Chon, E. Salhi

Section B
Ernest N. Morial Convention Center
Room 347

Shaping Activity through Structural Modification: From Small Molecules to Nanoparticles: A Symposium in honor of Professor Bing Yan

D.D. Dionysiou, V.K. Sharma, H. Zhou, *Organizers*
J. Chen, J. Liu, *Presiding*

8:00 Introductory Remarks.

8:15 ENVR 138. Toxicity of black phosphorus nanosheets (BPs). G. Qu, **G. Jiang**

8:40 ENVR 139. Multi-pollutants emissions and health exposure assessment from the burning of major agricultural straws in China. **J. Chen**, J. Li, Q. Li

9:05 ENVR 140. Controlled synthesis of atomically dispersed alloy shell of Au@PdAg nanoparticles by manipulating growth kinetics. Y. Lai, R. Liu, X. Zhou, **J. Liu**

9:30 ENVR 141. Simulating and predicting adsorption of organic pollutants on carbon nanomaterials. **J. Chen**, Y. Wang

9:55 Intermission.

10:15 ENVR 142. Clay mineral-based polymeric nanocomposites for heavy metal removal. **C. Wang**

10:40 ENVR 143. Mass spectrometry-based techniques for the investigation on toxicological mechanisms of bisphenol F in breast cancer xenografts. **Z. Cai**

11:05 ENVR 144. Transfer of antibiotic-resistance genes between different bacteria under light irradiation and at the interface of mineral. X. Chen, H. Yin, G. Li, **T. An**

11:30 ENVR 145. Chemical characterization of highly oxidized molecules (HOMs) in Linzhi, Tibet. L. Yao, **L. Wang**

Section C
Ernest N. Morial Convention Center
Room 348

Innovative Chemical & Material Approaches for Sustainable Water Purification

Adsorption

Cosponsored by CEI
J. Choe, J. Liu, D. Shuai, Y. Wang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 146. Effective adsorbents for toxic metal ions in water body based on macroporous polyvinyl alcohol-formaldehyde sponges. Y. Pan, K. Shi, Z. Liu, **X. Ji**

8:55 ENVR 147. Tailored cyclodextrins for environmental remediation of emerging perfluoroalkyl substances. **M.J. Weiss-Errico**, I. Ghiviriga, K.E. O'Shea

9:15 ENVR 148. Recovery of nitrogen and phosphorus nutrients via metal-exchanged zeolites. **M.J. Manto**, M.A. Keller, T. Pu, W. Liano, P. Xie, C. Wang

9:35 ENVR 149. Removal of nitrate and fluoride anions from aqueous solution using β-FeOOH and β-Fe_2O_3 modified biochar with fast adsorption kinetics . **N.W. Bombuwala Dewage**, A.S. Liyanage, C.U. Pittman, T. Mlsna

9:55 Intermission.

10:15 ENVR 150. New type of material derived from concrete sludge and its applications to pollution prevention processes: PAdeCS®. **A. Yamasaki**, A. Iizuka, T. Sasaki, H. Yoshida

10:35 ENVR 151. Novel carbon based smart filters for remediation of pharmaceutical contaminants. S.K. Misra, **I. Tripathi**, L. Dodgen, F. Ostadhossein, J. Scott, B. Sharma, W. Zheng, D. Pan

10:55 ENVR 152. Withdrawn.

11:15 ENVR 153. Composite of functionalized carbon nanotube and

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carbon nanofiber for improving water treatment. **Y. Han**, R. Li, C. Bruckner, J.R. McCutcheon, T.M. Vadas

11:35 ENVR 154. Polymeric functionalized clay composites for adsorption of trace contaminants in urban stormwater infiltration systems. **J. Ray**, M. Teixido, I. Shabtai, Y. Mishael, D.L. Sedlak

11:55 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 349

Environmental Chemistry Undergraduate Education in the Classroom, Laboratory & Beyond
Cosponsored by CHED
M. Berger, L.A. Welch, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 155. Establishing a long-term monitoring program of a local contaminated hotspot using a senior analytical environmental laboratory class. **S. Joudan**, A.O. De Silva, S.R. de Solla, J.C. D'eon

8:30 ENVR 156. Citizen science and college student partnership to assess stream health in the Charles River Watershed, Boston, MA. **L. Lobel**, E. Cianciola, M. Berger

8:50 ENVR 157. Semester-long course-based undergraduate research experience (CURE) in snow chemistry in the general chemistry laboratory. **N. May**, S. McNamara, J.P. Wolfe, J. Vernon, D. Goldberg, S. Wang, K. Kolesar, K.A. Pratt

9:10 ENVR 158. Multi-project development with focus on water quality in a four year undegraduate college. **G. Geme**

9:30 ENVR 159. Integration of environmental research into the freshman chemistry laboratory. **M. Karod**, B. Boschetti, E. Robinson, J.L. Goldfarb, M. Berger

9:50 Intermission.

10:05 ENVR 160. Multifunctional magnetic nanoparticles and electrochemical membrane filtration for sustainable biomass harvesting and water purification: A case study on incorporating research and sustainability concepts into classroom and laboratory teaching. **W. Zhang**

10:25 ENVR 161. CURE for climate change: Engaging the next generation with scientific computing and climate change data analysis. **A.K. Sharma**

10:45 ENVR 162. Undergraduate inorganic/materials research at UVa-Wise: Evaluating the roles of functional groups in zirconium-based metal-organic frameworks on stability, structural defects, and trace heavy metal capture. **T.A. Makal**

11:05 ENVR 163. Undergraduate international research at the food-energy-water nexus: Influence on research skills, research confidence, and cultural enrichment. B. Casad, **N. Mladenov**, M. Palomo, B. Pietruschka, C. Buckley

11:25 ENVR 164. Synthesis of fuel range chemicals from biomass using catalytic pathways. S. Ogozaly, A. Childs, **L.A. Welch**

11:45 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 350

Agro-Environmental & Energy Applications of Biochar/Hydrochar

Biochar/Hydrochar as Environmental Sorbents

N.D. Berge, C. Jeong, K. Ro, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 165. Biochar and its functionalization for agricultural and environmental applications. **J.J. Wang**

8:30 ENVR 166. Enhanced removal of nutrients and trace organic contaminants from urban runoff using biochar and manganese oxide-coated sand geomedia in capture, treatment, and recharge systems. **M. Teixido**, J. Charbonnet, N. Ashoori, R.G. Luthy, D.L. Sedlak

8:50 ENVR 167. Adsorption of pharmaceutical active compounds using activated carbons synthesized from herbaceous biomass. O. Oginni, **K. Singh**, L. McDonald

9:10 ENVR 168. Development of sustainable biochars for the aqueous remediation of organic and inorganic contaminants. **D. Mohan**, M. Patel, P. Singh, R. Kumar

9:30 ENVR 169. Biochar effect on the sorption-desorption and dissipation of 17 β-ethinylestradiol (ee2) in sandy and clay soils. **Z. Wei**

9:50 Intermission.

10:10 ENVR 170. Effect of feed source and pyrolysis conditions on properties and metal sorption by sugarcane biochar. **I.M. Lima**

10:35 ENVR 171. Properties of animal manure-derived hydrochars and pyrochars and their sorption of antimony (III) and cadmium (II). **L. Han**, K. Sun, B. Xing

10:55 ENVR 172. Coconut shell derived hierarchical carbon adsorbent for fluoride removal from aqueous solution: Synthesis, equilibrium, kinetics and thermodynamics studies. **R. Araga**, S. Kali, C. Sharma

11:15 ENVR 173. Adsorption of methylene blue onto activated carbon prepared from KOH-treated jamun (Syzygium cumini) seed: Equilibrium, kinetic and thermodynamic studies. **R. Araga**, P.P., C. Sharma

11:35 ENVR 174. Oxyanion sorption onto treated biochar surfaces. **S. Bakshi**, J.J. Pignatello

11:55 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 351

Aquatic Photochemistry

K.P. McNeill, *Organizer*
W. Arnold, S.G. Pati, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 175. Photochemical degradation of halogenated estrogens. R. Milstead, K. Nance, K. Tarnas, K. Egelhofer, **D.R. Griffith**

8:40 ENVR 176. Experimental and theoretical investigation of the UV/Vis absorption spectra of brominated 17β-ethynylestradiol and the implications for environmental photodegradation. **S.N. Eustis**, P. Brown

9:00 ENVR 177. Transformation rates and product formation of reactions of ionic liquid cations with photochemically produced radicals in natural and technical aquatic environments. **S.G. Pati**, W. Arnold

9:20 ENVR 178. Probing defluorination mechanisms for perfluorocarboxylic acids by a UV-mediated reduction system. **M.J. Bentel**, T. Brantner, R. Chavarria-Vivar, V. Coria, J. Liu

9:40 ENVR 179. Destruction of per- and polyfluoroalkyl substances (PFASs) in water sources impacted by aqueous film-forming foam (AFFF) using a photoreductive UV/sulfite process. **R. Tenorio**, J. Liu, X. Xiao, A. Maydanov, A. Maizel, C. Schaefer, C.P. Higgins, T.J. Strathmann

10:00 ENVR 180. Photolysis of 3-nitro-1,2,4-triazol-5-one (NTO): Mechanisms, products, and toxicity. **H. Schroer**, C.L. Just

10:20 Intermission.

10:30 ENVR 181. Excited triplet state of antibiotic norfloxacin interactions with dissolved natural organic matter: A laser spectroscopic study. **X. Niu**, E. Moore, J. Croue

10:50 ENVR 182. Photochemical transformation of pharmaceuticals in simulated aqueous environmental matrices using a high resolution mass spectrometric approach. **S. Wang**, T. Zeng

11:10 ENVR 183. Predicting transformation products from the direct photolysis of organic compounds in aquatic systems. **C. Yuan**, C. Tebes-Stevens, E.J. Weber

11:30 ENVR 184. Assessing the role of nitrate and nitrite in the transformation of wastewater-derived organic contaminants in sunlit waters. **R. Scholes**, C. Prasse, D.L. Sedlak

Section G
Ernest N. Morial Convention Center
Room 342

Novel Membrane-Based Technology for Water Purification & Desalination

Novel Thermal or Electro Membrane Processes

D. Jassby, B. Mi, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 185. Photothermal water purification membranes containing optically-tuned polydopamine particles embedded in bacterial nanocellulose. **Y. Jun**, Q. Jiang, H.G. Derami, D. Ghim, S. Cao, S. Singamaneni

8:30 ENVR 186. Waste heat driven membrane distillation for cost-effective produced water treatment in Pennsylvania. **O.R. Lokare**, S. Tavakkoli, G. Rodriguez, V. Khanna, R.D. Vidic

8:50 ENVR 187. Withdrawn.

9:10 ENVR 188. Withdrawn.

9:30 ENVR 189. Process modeling and economic optimization of a solar driven membrane distillation system for desalination. **S.E. Moore**, S.D. Mirchandani, V. Karanikola, T.M. Nenoff, R. Arnold, A.E. Saez

9:50 Intermission.

10:00 ENVR 190. Stable superhydrophobic desalination membranes using carbon nanotube networks. **Y. Dong**

10:30 ENVR 191. Combined catalytic/electrocatalytic nitrate reduction in a reactive electrochemical membrane. **B.P. Chaplin**, P. Gayen, J. Spataro, J.M. Cerrato, S. Avasara, A. Ali

10:50 ENVR 192. Comparison of Faradaic reactions in capacitive deionization (CDI) and membrane capacitive deionization (MCDI) water treatment processes. **D. He**, W. Tang, D. Waite

11:10 ENVR 193. Application of electro-membrane bioreactor (eMBR) for the removal of pharmaceuticals from wastewater. **B.B. Ensano**, V. Naddeo, L. Borea, M.G. de Luna, V. Belgiorno

11:30 ENVR 194. Novel membrane-electrode hybrid for advanced treatment of industrial wastewater effluents: Decontamination, disinfection, and anti-fouling performances. **K. Choo**, N. Mameda, H. Park, H. Park

Elucidation of Mechanisms & Kinetics on Surfaces

Theory

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Rafael Luque
Sponsored by CELL, Cosponsored by ENVR and I&EC

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

ACS-CEI Award for Incorporating Sustainability into Chemical Education
Sponsored by CHED, Cosponsored by CEI and ENVR

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Sponsored by GEOC, Cosponsored by ENVR

Contaminated Site Remediation through Microbial, Geological & Chemical Processes
Sponsored by GEOC, Cosponsored by

‡*Cooperative Cosponsorship*

ENVR

Wood-Based Materials for Energy & Water

Wood-Based & Related Materials

Sponsored by CELL, Cosponsored by ENFL, ENVR and MPPG

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 346

Physics & Chemistry of Water Treatment: Symposium in honor of Professor Desmond F. Lawler

Water Treatment: From Small Systems to Broad Ideas

J. Darby, H. Garcia, J.A. Nason, *Organizers*
L.E. Katz, N.B. Saleh, *Organizers, Presiding*

1:30 ENVR 195. Development and verification of a new model for competitive adsorption on multiple adsorbents. **M.M. Benjamin**, S. Modarresi

2:10 ENVR 196. Selecting the column configuration with the lowest replacement cost: Process analysis for small systems. **B. Dvorak**

2:30 ENVR 197. Pilot-scale evaluation of bicarbonate-form anion exchange for small water systems. **T.H. Boyer**, A. Ness

2:50 ENVR 198. Physics and chemistry of carbon dioxide as the driver for low-energy desalination and decontamination of impaired wastewater. **A.K. Sengupta**

3:10 Intermission.

3:30 ENVR 199. From water treatment to trophic transfer: Elements of particle aggregation modeling. **M. Wiesner**

4:10 ENVR 200. Looking back: Musing from an undergrad. **D. Niemeier**

4:30 ENVR 201.
No particle shall remain uncounted: Insights from the application of Coulter counter measurements to precipitative coagulation processes. **J.A. Nason**, L.E. Katz

4:50 ENVR 202. Raw water to reuse: Reflections and renewal. **D.F. Lawler**

Section B
Ernest N. Morial Convention Center
Room 347

Shaping Activity through Structural Modification: From Small Molecules to Nanoparticles: A Symposium in honor of Professor Bing Yan

H. Zhou, *Organizer*
D.D. Dionysiou, V.K. Sharma, *Organizers, Presiding*

1:30 ENVR 203. Sustainable applications of magnetic nanocatalysts and *N*-enriched carbonaceous materials. **R.S. Varma**

1:55 ENVR 204. Exposed facets determine surface reactivity of metal-based nanomaterials towards environmental and biological receptors. **W. Chen**, T. Zhang, L. Liu, P.J. Alvarez

2:20 ENVR 205. Formation, fate and toxicity of natural silver nanoparticles in the environment. **V.K. Sharma**

2:45 ENVR 206. Impact of advanced materials on the formation and toxicity of disinfection byproducts during drinking water chlorination. **C.M. Sayes**, V.K. Sharma

3:10 Intermission.

3:30 ENVR 207. Base modification of Bi_2WO_6 for enhanced photocatalytic activity under visible light. B. Ren, M. Nadagouda, **D.D. Dionysiou**

3:55 ENVR 208. Engineered Nano-TiO_2 in natural aquatic environment and effects on transformation of organic pollutants. **L. Zhu**, W. Wu

4:20 ENVR 209. Enhanced disinfection application of Ag-modified g-C3N4 compositeunder visible light. **S. Zhan**

4:45 ENVR 210. Surface modification regulates bioactivities of metallic nanoparticles. **Q. Zhou**, Y. Long, X. Zhao, G. Jiang

Section C
Ernest N. Morial Convention Center
Room 348

Innovative Chemical & Material Approaches for Sustainable Water Purification

Electrochemistry & Membrane Technology

Cosponsored by CEI
J. Choe, J. Liu, D. Shuai, Y. Wang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 211. Electrochemical activation of nitrate: Simultaneous removal of nitrate and organic pollutants. **K. Lee**, H. Lee, M. Kim, C. Lee

1:55 ENVR 212. Simultaneous coagulation and inactivation during iron electrochemical treatment for virus control. **K. Kim**, S. Chellam

2:15 ENVR 213. Electrochemically mediated regeneration of ionic liquids (EMRIL) for heavy metal removal and water disinfection. **S. Voskian**, P. Brown, C. De La Fuente-Nunez, T. Hatton

2:35 ENVR 214. Redox-responsive gels in asymmetric Faradaic systems for electrochemically mediated separations organic pollutants from water. **Y. Ren**, T. Hatton

2:55 Intermission.

3:15 ENVR 215. Electrochemical reactions and processes in membrane-based water treatment: Challenges and opportunities. **D. Jassby**

4:15 ENVR 216. Enhancing counter-ion adsorption efficiency in capacitive deionization with charged polysaccharide binders. **M. del Cerro**, M. Kim, S. Hand, R.D. Cusick

4:35 ENVR 217. Development of a novel separation and recycle process of boron in waste water with bipolar membrane electrodialysis. **A. Yamasaki**, M. Noguchi, Y. Nakamura, T. Shoji

4:55 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 349

Redox & Interfacial Dynamics Among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients
Cosponsored by GEOC
Y. Hu, T. Zeng, *Organizers*
J.M. Cerrato, Z. Wang, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 218. Electron transfer between microorganisms and Fe(III) minerals mediated by redox-active biochar and natural organic matter. **A. Kappler**, Z. Yang, Y. Bai, R. Kretzschmar, T. Borch

2:10 ENVR 219. Mechanistic characterization of iron-organic matter interactions. **T. Borch**, E. Daugherty, B. Gilbert, C. Pallud, R. Young, G. Lobo, P.S. Nico, A. Kappler

2:45 ENVR 220. Effect of sulfide on the structure and stability of NOM-Fe(III) colloids under anoxic conditions. **P. Liao**, S. Yuan, C. Liu

3:05 ENVR 221. Nature and magnitude of strong oxidant formation during oxygen-mediated iron(II) monosulfide oxidation. **C.J. Miller**, J. He, Y. Chen, R. Collins, D. Waite

3:25 Intermission.

3:40 ENVR 222. Redox dynamic iron mineralogy and its effect on uranium transformations. **K.M. Kemner**, M. Boyanov, D. Latta, B. Mishra, E.J. O'Loughlin, M. Scherer, S. Yan

4:15 ENVR 223. Metastable sulphur species at iron mineral surfaces. **S. Peiffer**, C. McCammon, M. Wan, C. Schroeder

4:50 ENVR 224. Sequestration of phosphate by Fe(II)-Fe(III) green rust in anoxic sediments: Implication for eutrophication control. **L. Fang**

5:10 ENVR 225. Withdrawn.

Section E
Ernest N. Morial Convention Center
Room 350

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern
Cosponsored by ANYL and CEI
Y. Men, *Organizer*
L.M. Blaney, A.J. Hernandez, A. Heyden, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 226. Developing pre-concentration methods to address the challenge of treating CECs at extremely low concentration: Using synthetic estrogen 17β-ethinylestradiol as an example. C. Ng, L. Lu, R. Wang, **B. Cao**

1:55 ENVR 227. Quantification and comparison of free, conjugated, and halogenated estrogens in effluent from several wastewater treatment plants in northwestern Oregon. **C.P. Hutchinson**, L. Vine, L. Olson, D.R. Griffith

2:15 ENVR 228. Occurrence and distribution of a wide range of hormones and UV-filters in water, sediment, and coral (*Porites* spp.) from Hawaii. **K. He**, E. Hain, C. Mitchelmore, A. Heyes, M. Gonsior, L.M. Blaney

2:35 ENVR 229. Using high resolution mass spectrometry for identification and treatment assessment of novel organic contaminants in urban stormwater runoff. **E.P. Kolodziej**, K. Peter, C. Wu

3:05 Intermission.

3:25 ENVR 230. Analytical advances for the quantification and identification of emerging per- and polyfluoroalkyl substances in water: Looking beyond EPA 537. **T. Anumol**, R. Hindle, B. Clarke

3:45 ENVR 231. Detection and treatment of per- and polyfluorinated compounds in Cape Fear River Basin, North Carolina surface water. **Z. Hopkins**, M.J. Weiss-Errico, K.E. O'Shea, J. McCord, M. Strynar, A. Lindstrom, D. Knappe

4:05 ENVR 232. Spatial analysis of contaminants of emerging concern in Chesapeake Bay water, sediment, and oysters. K. He, E. Hain, A. Timm, E. Woytowitz, M. Tarnowski, **L.M. Blaney**

4:25 ENVR 233. Picolinic acid attenuation and microbial community effects in Alaskan soils, biotic/abiotic treatment, and insights into plant mobility. **P.L. Tomco**, K. Duddleston, S. Seefeldt

Section F
Ernest N. Morial Convention Center
Room 351

Aquatic Photochemistry

W. Arnold, *Organizer*
K.P. McNeill, S.G. Pati, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 234. When ROS are not ROS: The effect of salts on the degradation of protein. W. Mitch, Y. Komaki, **J. Choe**

1:55 ENVR 235. Impact of higher order nucleic acid structure on reactivity with UV_{254}. **Z. Qiao**, P. Chang, K. Wigginton

2:15 ENVR 236. Food dye photosensitizers for solar disinfection and safety indication of drinking water. **E. Ryberg**, C. Chu, J. Kim

2:35 ENVR 237. Withdrawn.

2:55 ENVR 238. Differentiating the inhibitory effects of natural organic matter constituents on photocatalytic treatment processes. **S. Snow**, M. Maghsoodi, C. Jacquin, V. Tarabara, G. Lesage, M. Heran

3:15 Intermission.

3:25 ENVR 239. Phototoxicity of dicloran to marine and freshwater organisms. **E.N. Vebrosky**, W. Xu, L.M. Basirico, C. Lutz, K.L. Armbrust

3:45 ENVR 240. Night and day: Chemicals interactions between photoactive nanomaterials enhance bacterial stress under irradiation. **C. Wilke**, J. Gaillard, K.A. Gray

4:05 ENVR 241. Quantum dots dissolution in the aqueous environment. **P. Paydary**, P. Larese-Casanova

4:25 ENVR 242. Release and toxicity of fragments generated during the photodegradation of quantum dot

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polymer composites. **M.J. Gallagher**, J.T. Buchman, T.A. Qiu, B. Zhi, T. Curry, Z. Rosenzweig, C.L. Haynes, H. Fairbrother

4:45 ENVR 243. Surface property changes of cerium oxide nanoparticles in the presence of UV/H_2O_2 and natural organic matter. **X. Wu**, C. Neil, D. Kim, H. Jung, Y. Jun

Section G
Ernest N. Morial Convention Center
Room 342

Novel Membrane-Based Technology for Water Purification & Desalination

Novel Membrane & Processes

D. Jassby, B. Mi, *Organizers, Presiding*

1:30 Introductory Remarks.

1:40 ENVR 244. Comparison of liquid membranes for selectivity of rare earth elements from coal ash leachates. R. Smith, **H. Hsu-Kim**, M.R. Wiesner

2:00 ENVR 245. Novel thin-film composite nanofiltration membranes with covalent organic framework active layer. **G. Levato**, A.R. Corcos, W. Dichtel, A. Livingston, B.J. Marinas

2:20 ENVR 246. Novel polyimide membranes derived from β-cyclodextrin for environmental remediation applications. **E. Leonhardt**, K. Gupta, T. Williams, K.L. Wooley

2:40 ENVR 247. Enhanced degradation of unregulated organic micropollutants via heterogeneous photo-Fenton reactions and hybridization with ceramic membrane filtration. **W. Zhang**, G. Zhang, S. Sun, H. Yao

3:00 Intermission.

3:10 ENVR 248. Self-sustaining polymer nanofilm on a buckypaper scaffold for chemical separations. **H. Park**

3:40 ENVR 249. Potential of ceramic and polymeric nanofiltration membranes in the reuse of abandoned coal mine drainage. **S. Wadekar**, R.D. Vidic

4:00 ENVR 250. Using ion exchange membranes to recover phosphorus from wastewater. **U. Shashvatt**, H. Aris, S. Musa, C. Portner, L.M. Blaney

4:20 ENVR 251. Predicting RO removal of toxicologically relevant unique organics. **D. Minakata**, M. Zhang, L. Breitner, K. Howe

4:40 ENVR 252. IR fluorescent probe for water-based agricultural nutrients. **M. Mohammadizadeh**, H.A. Stretz, R. Mu

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Lignin: From Fundamentals to New Materials & Applications

Fundamental Understanding of Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Sponsored by GEOC, Cosponsored by ENVR

Nexus of Food, Energy, & Water: Adapting to Future Challenges
Sponsored by MPPG, Cosponsored by AGFD‡, ENFL‡ and ENVR‡

Contaminated Site Remediation through Microbial, Geological & Chemical Processes
Sponsored by GEOC, Cosponsored by ENVR

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Value Added from Agricultural Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

Undergraduate Research Posters

Environmental Chemistry

Sponsored by CHED, Cosponsored by ENVR and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
S.O. Obare, *Organizer*

8:00–10:00

506-507, 511-515, 519-520, 522, 524, 526, 528, 533, 536-541, 543, 546-547, 552-554, 556-561, 563-567, 572, 574, 578-579, 581-583, 595-597, 603, 607, 612, 614, 623, 627, 637-639, 643-645, 648-649, 651, 654, 658, 660-661, 664-665, 669-670, 672-675. See subsequent listings.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 346

Physics & Chemistry of Water Treatment: Symposium in honor of Professor Desmond F. Lawler

Innovative Treatment Applications

L.E. Katz, J.A. Nason, N.B. Saleh, *Organizers*
J. Darby, H. Garcia, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 253. UV photolysis of chloramines for potable water reuse. S. Patton, K.P. Ishida, **H. Liu**

8:25 ENVR 254. Tailored graphitic carbon nitride: Smart design of visible-light-responsive photocatalyst to achieve sustainable water treatment. **D. Shuai**

8:45 ENVR 255. Enveloped virus inactivation by UV and chlorine disinfection. **Y. Ye**, K. Wigginton

9:05 ENVR 256. Assessing the impact of wildfires on source water quality and treatment. **F.L. Rosario**

9:25 ENVR 257. Effective removal of trace Tl from drinking water by conventional processes enhanced by $nMnO_2$. **X. Huangfu**, L. Sun, J. Song, C. Ma, R. Huang, Y. Xu, H. Wang

9:45 Intermission.

10:00 ENVR 258. Redox activity alteration of transformed CeO_2 NPs upon adsorption of ionic arsenic. **X. Bi**, P.K. Westerhoff

10:20 ENVR 259. Permanganate as a treatment strategy for algal toxins. **J.R. Laszakovits**, A. Mackay

10:40 ENVR 260. Technical feasibility of inland desalination using zero discharge desalination. **M. Cappelle**, W. Walker, T. Davis

11:00 ENVR 261. Hydrolysis of the Zika pesticide naled: Kinetics and mechanistic investigation. **A. Abdullah**, K.E. O'Shea

11:20 ENVR 262. Mapping the reactions in a single zero-valent iron nanoparticle. **L. Ling**, W. Zhang

11:40 ENVR 263. Refining the parameterization of engineered nanomaterial heteroaggregation within aquatic environments: The relative influence of surface coating functionality. **M.C. Surette**, J.A. Nason

Section B
Ernest N. Morial Convention Center
Room 347

Shaping Activity through Structural Modification: From Small Molecules to Nanoparticles: A Symposium in honor of Professor Bing Yan

D.D. Dionysiou, V.K. Sharma, *Organizers*
H. Zhou, *Organizer, Presiding*
W. Zhang, *Presiding*

8:15 ENVR 264. Pot-economic synthesis and asymmetric organocatalysis. **W. Zhang**

8:40 ENVR 265. Application of combinatorial approach for developing new methodologies in hetero-cyclic compound synthesis. X. Liu, **Y. Han**

9:05 ENVR 266. Bi- and tri-orthogonal linkers for bioconjugation. **F. Albericio**, B. de la Torre

9:30 ENVR 267. Reaction-based smart ionic liquids. **Y. Chang**, Y. Chu

9:55 Intermission.

10:15 ENVR 268. NF-κB-regulated microRNA-574-5p underlies synaptic and cognitive impairment in response to atmospheric $PM_{2.5}$ aspiration. **N. Sang**

10:35 ENVR 269. Correlating the nanoparticles' biological effects with their physicochemical properties. X. Bai, **H. Zhou**, B. Yan

10:55 ENVR 270. Tuning cell autophagy by diversifying carbon nanotubes' surface chemistry. **L. Wu**, B. Yan, Y. Zhang

11:15 ENVR 271. Susceptibility of overweight mice to Ag NPs or ZNPs/Pb^{2+} exposures. **J. Jia**, B. Yan

11:35 ENVR 272. Polyvinylidene fluoride micropore membranes as solid phase extraction disc for preconcentration of nanoparticulate silver in environmental waters. **X. Zhou**

Section C
Ernest N. Morial Convention Center
Room 348

Innovative Chemical & Material Approaches for Sustainable Water Purification

Photocatalysis

Cosponsored by CEI
J. Choe, J. Liu, D. Shuai, Y. Wang, *Organizers, Presiding*

8:45 Introductory Remarks.

8:50 ENVR 273. UV photocatalysis of recalcitrant organics in a fluidized-bed tubular reactor. **G.J. Rincon**

9:10 ENVR 274. Study of the photochemical and adsorptive properties of NOM grafted iron oxide nanoparticles for the potential remediation of toxic arsenic from water. **M. Rashid**, K.E. O'Shea

9:30 ENVR 275. Enhanced visible light-induced photocatalytic activity of surface-modified CeO_2 with metal particles. **L. Wang**, Y. Wang

9:50 ENVR 276. Discrete buoyant photocatalysts for interfacial pollutants. **M.J. Nee**, B.R. John, K.A. Steward

10:10 Intermission.

10:30 ENVR 277. Visible-light-responsive photocatalystic graphitic carbon nitride for antimicrobial applications. **D. Shuai**

10:50 ENVR 278. Growth of UiO-66 metal-organic framework onto a cotton fabric and its use as a functional micropollutant filter. **M. Schelling**, E. Otal, J.P. Hinestroza

11:10 ENVR 279. Photocatalytic degradation of PFAS by $BiPO_4$ microparticles. **E.L. Cates**, S. Sahu

11:30 ENVR 280. PEI functionalized graphene oxide for enhanced sorption and rapid photoreduction of chromium (VI). **C. Kim**, S. An, J. Fortner

11:50 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 349

Redox & Interfacial Dynamics Among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients
Cosponsored by GEOC
J.M. Cerrato, Z. Wang, *Organizers*
Y. Hu, T. Zeng, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 281. Quantification of mercury biomethylation potential in sediments. **H. Hsu-Kim**, U. Ndu, G.A. Christensen, D. Elias

‡*Cooperative Cosponsorship*

8:40 ENVR 282. Chemodiversity of dissolved organic matter in anaerobic sediments with a special focus on non-volatile dissolved organic sulfur. **M. Gonsior**, J. Luek, A. Heyes, L. Lapham, L. Powers, P. Schmitt-Kopplin

9:15 ENVR 283. Sulfur and iron cycling at the sediment-root interface of freshwater wetland plants: Life-cycle controlled redox transitions. S. Lafond-Hudson, **N.W. Johnson**, J. Pastor, B. Dewey

9:35 ENVR 284. Effect of reducing and re-oxidizing conditions on metal mobility in sediments from the Animas River. **L. Rodriguez Freire**, A. Overbey, C.M. Saup, A. Ali, M.J. Wilkins, J.M. Cerrato

9:55 Intermission.

10:10 ENVR 285. Reactions of nanoscale zero-valent iron (nZVI) with heavy metals: 3D visualization. **W. Zhang**, L. Ling

10:45 ENVR 286. Aqueous-phase reduction of nitroaromatic compounds (NACs) by sulfide mediated by carbonaceous materials. C. Wei, H. Fu, X. Qu, **D. Zhu**

11:20 ENVR 287. Sulfidation of iron-based materials for contaminant removal: The diverse effects of processes and operational variables. **D. Fan**, P.G. Tratnyek, Y. Lan, C. Xu

11:40 ENVR 288. Sulfide removal by iron-bearing minerals in mining waste streams. **J. Voelz**, J. Daire, C. Chun, N.W. Johnson, R. Penn

Section E
Ernest N. Morial Convention Center
Room 350

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern
Cosponsored by CEI
Y. Men, *Organizer*
L.M. Blaney, A.J. Hernandez, A. Heyden, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 289. Determining the kinetics of oxidative radical reactions with organophosphate/brominated flame-retardants under advanced oxidation process conditions. **M. Chin**, S.P. Mezyk

8:55 ENVR 290. Advanced oxidation process removal of oxidized nitrosamines (nitramines) from treated wastewaters. **R.N. Tran**, J.J. Kiddle, S.P. Mezyk

9:15 ENVR 291. Radical-induced degradation of estrogenic steroids in treated wastewaters. **J. Gleason**, A. Lechner, E. Holland, S.P. Mezyk

9:35 ENVR 292. Can hydrogen peroxide enhance 1,4-dioxane oxidation by ozone in surface water and lower bromate formation? **N. Kotlarz**, Z. Hopkins, D. Knappe

9:55 ENVR 293. Challenges of advanced wastewater treatment to abate CECs. **C. McArdell**, M. Boehler, M. Bourgin, J. Fleiner, A. Joss, A. Meier, H. Siegrist, U. von Gunten

10:25 Intermission.

10:40 ENVR 294. Bromamine species reactions under advanced oxidation process conditions. **M.V. Luong**, A. Lechner, S.P. Mezyk

11:00 ENVR 295. Improving activity and stability of perchlorate reduction catalyst with rational ligand design for the rhenium complex reaction site. **C. Ren**, J. Liu

11:20 ENVR 296. Ferrate(VI) oxidation of pharmaceuticals in hydrolyzed urine: Enhancement effects from ammonia, bicarbonate, and creatinine. **C. Luo**, V.K. Sharma, C. Huang

11:40 ENVR 297. N-TiO_2/CdS nano-composite: Synthesis, characterization, and photocatalytic degradation of textile dye wastes. H. Hiluf, T. Abi, **S.M. Abegaz**

Section F
Ernest N. Morial Convention Center
Room 351

From Sewage to Sustainable Energy: Potential Pollution Issues from Production & Application Pathways

Financially supported by EuCHeMS
S. Chae, W. Giger, R. Kallenborn, A. Torrents, *Organizers, Presiding*

8:00 Introductory Remarks.

8:10 ENVR 298. Withdrawn.

8:30 ENVR 299. Withdrawn.

8:50 ENVR 300. Simultaneous reduction of ammonia toxicity and recovery of nutrients in mixed liquor of anaerobic digester. **H. Kim**, T. Antukh, D. Lee, J. Baek

9:10 ENVR 301. Impact of solids stabilization processes on energy production and polybrominated diphenyl ethers content. **N.A. Andrade**, A. Torrents, M. Ramirez

9:30 ENVR 302. Influence of anaerobic digestion with and without thermal hydrolysis pretreatment on concentrations of endocrine disrupting compounds and their transformation products in wastewater sludge. **D.L. Armstrong**, S.J. Fischer, R.M. Lupitskyy, C.P. Rice, M. Ramirez, A. Torrents

9:50 Intermission.

10:00 ENVR 303. European Association of Chemical and Moleclar Sciences (EuCheMS) and its Division of Chemistry and the Environment. **W. Giger**

10:20 ENVR 304. Identification of novel chlorinated and hydrogenated polyfluoroalkyl ether sulfonates in sewage sludge by high-resolution mass spectrometry. **T. Ruan**, G. Jiang

10:40 ENVR 305. Occurrence and fate of neonicotinoid pesticides (NEOs) in wastewater treatment plants in China. **T. Zhang**

11:00 ENVR 306. Not just what but when: Stage-specific effects of emerging contaminants in the early development of marine organisms. **C. Torres**, K. Ramos-Torres, R. Rahimoff, G.N. Cherr

11:20 ENVR 307. Withdrawn.

11:40 ENVR 308. Transformation of heavy metals during (hydro)thermal treatments of sewage sludges: Implications for resource recovery. **R. Huang**, B. Zhang, E. Saad, E.D. Ingall, Y. Tang

Section G
Ernest N. Morial Convention Center
Room 342

Great Achievements in Environmental Science & Technology

Financially supported by Environmental Science & Technology and Environmental Science & Technology Letters
N. Barsamian, B.E. Logan, D.L. Sedlak, *Organizers*
D. Sedlak, *Presiding*

8:30 Introductory Remarks.

8:35 ENVR 309. Engineered nanoparticles and dissolved organic matter: Are we missing the forest for the trees? **M. Scheringer**

9:00 ENVR 310. Desalinated drinking water: What chemicals are we drinking and how safe is it? **S.D. Richardson**, A.A. Cuthbertson, H.K. Liberatore, D. Westerman, M.J. Plewa, M. Gonsior, C. Mitchelmore, A. Heyes, J. Croue, W. El-Shorbagy

9:25 ENVR 311. Materials for next generation desalination and water purification membranes. **M. Elimelech**

9:50 ENVR 312. Stuck in the muck: Historical insights into emerging contaminants from sediment cores. **W. Arnold**

10:15 Intermission.

10:35 ENVR 313. Halogen radicals promote the photodegradation of microcystins in estuarine systems. W. Mitch, **K.M. Parker**, A. Ghadouani, E. Reichwaldt

11:00 ENVR 314. Update on occurrence and control of legacy and emerging perfluoroalkyl substances in North Carolina. **M. Sun**, E. Arevalo, M. Strynar, A. Lindstrom, D. Knappe

11:25 ENVR 315. Science on Ice: Shedding light on arctic halogen photochemistry. **K.A. Pratt**

11:50 Concluding Remarks.

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, ENVR‡, INOR, PMSE‡ and PRES‡

Water Supply Safety
Sponsored by CHAS, Cosponsored by CCS, CTA and ENVR

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

Lignin: From Fundamentals to New Materials & Applications

Advances in Lignin Characterization

Sponsored by CELL, Cosponsored by ENVR and POLY

Cheminformatics Resources & Software Tools Supporting Environmental Chemistry
Sponsored by CINF, Cosponsored by COMP and ENVR

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Sponsored by GEOC, Cosponsored by ENVR

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Ning Yan
Sponsored by CELL, Cosponsored by ENVR and I&EC

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Sponsored by GEOC, Cosponsored by AGFD, AGRO and ENVR

Biobased Water Purification System Approaches
Sponsored by CELL, Cosponsored by AGFD, CHAS and ENVR

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Food, Water & Energy from Sustainable Crops

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Enabling Fundamental Advances in Catalysis & Surface Science

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 346

Science & its Perception: Climate Change, Nicotine, Pollution & Other Emerging Topics in the Crosshair
Cosponsored by CEI‡
S.O. Obare, E. Schoffers, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 316. Withdrawn

2:00 ENVR 317. Climate disruption has created a new world: Discuss. **J.A. Bell**

2:25 ENVR 318. eCLEAR, climate science literacy tools for all. **G.P. Foy**, K.E. Peterman

2:50 ENVR 319. Lost in translation: How mass media influence climate change (in) action and why we should care about science communication. **E. Schoffers**

3:15 Intermission.

3:25 ENVR 320. The real crisis with Flint's water: It was preventable and can

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happen to you! **M.R. Wilhelm**

3:45 ENVR 321. How an interdisciplinary, environmental narrative of natural history promotes communication of controversial topics: Evolution, origin of life, and climate history. **B.J. McFarland**

4:05 ENVR 322. Understanding the rationale of climate-change denial. **G.M. Bodner**

4:30 ENVR 323. Global warming is unequivocal: We must learn how to communicate the science of climate change to ourselves and also to non-science audiences. **B.Z. Shakhashiri**

4:55 Panel Discussion .

Section B
Ernest N. Morial Convention Center
Room 347

Shaping Activity through Structural Modification: From Small Molecules to Nanoparticles: A Symposium in honor of Professor Bing Yan

D.D. Dionysiou, V.K. Sharma, H. Zhou, *Organizers*
S. Liu, H. Zhu, *Presiding*

1:30 ENVR 324. Knocking on placenta's door: Engineered nanoparticles at the human placental barrier. **P. Wick**, T. Buerki-Thurnherr

1:55 ENVR 325. Low-dose exposure of graphene oxide compromises cellular priming state that predisposes macrophages to metal toxicity. **S. Liu**

2:20 ENVR 326. Virtual nanostructure simulation (VINAS): A toolbox to quantify nanomaterial structures for intelligent modeling and rational material design. W. Wang, A. Sedykh, X. Yan, B. Yan, **H. Zhu**

2:45 ENVR 327. Photochlorinated fullerene increase cytotoxicity towards macrophage J774 via acting as SOD and electron-transfer mediator. **C. Zhang**, Q. Zhang

3:10 Intermission.

3:25 ENVR 328. Toxicity of rare earth nanomaterials in macrophages. J. Gao, **G. Qu**

3:50 ENVR 329. Graphene oxide nanosheets elicit neurotoxicity. **X. Hu**

4:15 ENVR 330. Effects of titanium dioxide and zinc oxide nanoparticles on disinfection byproduct formation in synthetic freshwater. **C. Gray**, **V.K. Sharma**, L.H. Cizmas

4:40 ENVR 331. Systematic exploration of nano-bio interactions for water safety and human health. **B. Yan**

5:05 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 348

Innovative Chemical & Material Approaches for Sustainable Water Purification

Oxidation & Sensor

Cosponsored by CEI
J. Choe, J. Liu, D. Shuai, Y. Wang, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 332. Effect of organic ligands on oxidative degradation of chlorophenolic compounds (CP) with modified-Fenton process using pyrite as the catalyst. **C. Kantar**, O. Oral, N.A. Oz

1:55 ENVR 333. Selectively degradation of organic pollutants in the homogeneous or heterogeneous non-radical reactions. **M. Long**, P. Hu, H. Su

2:15 ENVR 334. Decomposition of perfluorinated chemicals by nanoscale zerovalent iron conjugated with common oxidants. **A. Parenky**, N. Souza, H. Choi

2:35 ENVR 335. Impact of chitosan and polyacrylamide on formation of carbonaceous and nitrogenous disinfection by-products. **Z. Li**, T. Chen, Y. Xie, W. Xu

2:55 Intermission.

3:15 ENVR 336. Nanocellulose based nanocomposites for environmental sensing. **P.J. Vikesland**

3:55 ENVR 337. Reactivity of trichloramine with organic species under AOP conditions. **L. Watts**, S.P. Mezyk

4:15 ENVR 338. Structure modification of nature organic matter after microwave, ferrate and their combination processes. **X. Zhang**, V. Sharma

4:35 ENVR 339. Removal of perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) using two dimensional transition metal dichalcogenides. Y. Tian, **I. Chowdhury**

4:55 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 349

Redox & Interfacial Dynamics Among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients
Cosponsored by GEOC
Y. Hu, Z. Wang, T. Zeng, *Organizers*
J.M. Cerrato, *Organizer, Presiding*
Z. Wang, *Presiding*

1:30 Introductory Remarks.

1:35 ENVR 340. Intimate and complex coupling of carbon and iron cycles within terrestrial systems. **S.E. Fendorf**, M. Keiluweit, M.V. Schaefer, Y. Masue-Slowey, O. Chadwick

2:10 ENVR 341. Metabolomics-resolved nutrient-dependent carbon fluxes in a soil bacterium: Cellular insights on coupled iron and carbon cycles. **L. Aristilde**

2:45 ENVR 342. Formation and reactivity of ferrihydrite-organic carbon-calcium co-precipitate complexes. **D. Adhikari**, T.D. Sowers, J. Stuckey, D.L. Sparks, Y. Yang

3:05 ENVR 343. Robust spatial analysis of sequestered metals in an arid Southern California bioswale: Relating sequestration efficiency to preferential metal binding in soil. **Z. Evans**, H. Van Ryswyk, M. Los Huertos, T. Srebotnjak

3:25 Intermission.

3:40 ENVR 344. Multiscale investigation of microbial oxidation of soil organic carbon and effective integration of pore-scale mechanisms into macroscopic models. **C. Liu**

4:15 ENVR 345. Nitrate-reducing As(III) oxidizers and nitrate-reducing Fe(II) oxidizers in flooded paddy soil revealed by metagenomic binning. **F. Li**, X. Li, S. Li, M. Hu, T. Liu

4:50 ENVR 346. Enhanced biological sulfate reduction coupled to iron electrolysis in a flow-through bioelectrochemical reactor. **T. Deen**, **D.C. Takaki**, D.S. Jones, C. Chun

5:10 ENVR 347. Chemical regeneration of Mn-oxide coated sand for oxidation of organic stormwater contaminants. **J. Charbonnet**, D.L. Sedlak

Section E
Ernest N. Morial Convention Center
Room 350

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern
Cosponsored by CEI
Y. Men, *Organizer*
L.M. Blaney, A.J. Hernandez, A. Heyden, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 348. Maize root culture based model system for studying biotransformation of contaminants of emerging concerns. **M. Gautam**, M. Elhiti, I.S. Fomsgaard

1:55 ENVR 349. Adaptation of microbial communities to emerging pollutants in chemostat systems. B. Poursat, M. Braster, R. Helmus, R. van Spanning, P. de Voogt, **J. Parsons**

2:15 ENVR 350. Do the microbial communities growing on microplastics present another hazard? K. Parrish, **N. Fahrenfeld**

2:35 ENVR 351. Advanced transition metal based hierarchical porous materials for the equilibrium and dynamic adsorption of contaminants of emerging concern including metabolites. **A.J. Hernandez**, K. Ortiz-Martinez, B. Fernandez-Reyes, J.C. Muñoz-Senmache

2:55 Intermission.

3:15 ENVR 352. Investigating the metabolic fate of 1H-perfluoroalkanes. **S. Joudan**, S.A. Mabury

3:35 ENVR 353. Occurrence and fate of emerging organic contaminants in wastewater treatment processes with an enhanced nitrification step. **Y. Xing**, Y. Yu, Y. Men

3:55 ENVR 354. Challenges and solutions for the removal of pharmaceuticals from wastewater: The use of fungal treatment and integrated membrane systems. **D. Barcelo**, D. Lucas, M. Llorca, M. Villagrasa, **A. Jaen**, M. Stefani, J. Mamo, H. Monclus, Q. Comas, I. Rodriguez-Roda, M. Garcia-Galán, D. Dolar, G. Caminal, M. Sarra, M. Badia, F. Castellet, J. Mir Tutusaus, T. Vicent, S. Rodriguez-Mozaz

4:15 ENVR 355. Long-term development of bacterial resistance against disinfectants: Hypochlorite vs. ferrate. **S. Daer**, K. Ikuma, J. Goodwill, H. Truong

Section F
Ernest N. Morial Convention Center
Room 351

Evolving Chemical Hazard Evaluation Strategies to Address Compliance under the New Toxic Substances Control Act (TSCA)
Cosponsored by CHAL and CHAS
T. Lewandowski, J. Rice, *Organizers, Presiding*

1:30 ENVR 356. Chemical safety evaluation challenges of the Lautenberg Chemical Safety Act. **T. Lewandowski**, J. Rice

1:50 ENVR 357. Strategies for incorporating in silico and in vitro approaches into the safety evaluation of existing and new products. **P. Spencer**

2:10 ENVR 358. Fish liver microtissues for aquatic toxicology: Integrating morphological and molecular responses for *in vitro* assessment of environmental pollutants. **A. Rodd**, A. Kane

2:30 ENVR 359. Development of a tool for systematic integration of traditional and new approach methods for prioritizing chemical lists. **A.J. Williams**, R. Judson, C. Grulke, R. Thomas

2:50 ENVR 360. Applying chemical space analysis to select compounds for targeted *in vitro* methods. **C.I. Nicolas**, K. Mansouri, S. Haider, M. Yoon, P.D. McMullen, K. Phillips, J. Wambaugh, A. Tropsha, R. Clewell, H. Clewell

3:10 Intermission.

3:30 ENVR 361. Generalised read-across GenRA, research, implementation and practical application. **G. Patlewicz**, G. Helman, I. Shah

3:50 ENVR 362. Does one size fit all? Tailoring read-across methodology based on endpoint-specific criteria. **J. Rice**, J.M. Cohen, T. Lewandowski

4:10 ENVR 363. In silico modeling as a tool to aid design safer preservatives for consumer products. **D. Faulkner**, H.L. Buckley, W.M. Hart-Cooper, J.H. Kim, L. Cheng, K.L. Chan, C.D. Vulpe, W.J. Orts, S. Amrose, M.J. Mulvihill

4:30 ENVR 364. Tiered risk-based safety evaluation for a 21st century TSCA. **R.A. Becker**

4:50 ENVR 365. Use of alternative methods to assess health and environmental hazards. **A. Tveit**

5:10 Discussion.

Section G
Ernest N. Morial Convention Center
Room 342

ACS Award Symposium for Creative Advances in Environmental Science & Technology
Cosponsored by WCC
Financially supported by AEESP
S.O. Obare, *Organizer*
V.F. McNeill, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 366. Aqueous atmospheric chemistry: From clouds to aerosol particles. **V.F. McNeill**

2:05 ENVR 367. Climate impact of secondary organic aerosols on cirrus clouds. **J. Penner**, C. Zhou

2:35 ENVR 368. Chemistry of atmospheric brown carbon. **A. Laskin**

3:05 Intermission.

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3:20 ENVR 369. Direct measurements of aerosol acidity: Spectroscopic and colorimetric methods. **A.P. Ault**

3:50 ENVR 370. Award Address (ACS Award for Creative Advances in Environmental Science and Technology Sponsored by the ACS Division of Environmental Chemistry and the ACS Publications journals Environmental Science & Technology and Environmental Science & Technology Letters). Liquid water and secondary organic aerosol formation: Insights from diverse environments. **B. Turpin**

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Lignin: From Fundamentals to New Materials & Applications

Lignin Valorization in Biorefineries

Sponsored by CELL, Cosponsored by ENVR and POLY

Cheminformatics Resources & Software Tools Supporting Environmental Chemistry
Sponsored by CINF, Cosponsored by COMP and ENVR

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Silica/Alumina Surfaces & the Electrical Double Layer

Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Sponsored by GEOC, Cosponsored by AGFD, AGRO and ENVR

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

Sustainable Production & Processing of Agricultural Crops: The Food, Energy, Water Nexus

Biomaterials Processing

Sponsored by CELL, Cosponsored by AGFD, ENFL, ENVR and MPPG

R&D in the Chemical Catalysis for Bioenergy Consortium
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Enabling Fundamental Advances in Catalysis & Surface Science
Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 346

Novel Concepts in the Role of Chemistry in the Food, Energy & Water Nexus
Cosponsored by MPPG
S. Ahuja, S. Chae, *Organizers*
I. Chowdhury, D.D. Dionysiou, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 371. Role of chemistry in food-energy-water nexus research. **B.L. Schottel**

8:35 ENVR 372. Unmet challenges in developing energy efficient processes for reuse of municipal wastewater in large metropolis. **A.K. Sengupta**

9:05 ENVR 373. Withdrawn.

9:25 ENVR 374. Electrochemical reactivity of carbonaceous materials for water treatment and energy recovery. **R. Doong**, P. Chang, C. Hsu

9:45 ENVR 375. Withdrawn.

10:05 Intermission.

10:20 ENVR 376. Evaluating the potential of phosphorous recovery from corn-ethanol plants using chemical precipitation and enzymatic transformation. **N. Sharma**, V. Singh, R.D. Cusick

10:40 ENVR 377. *In situ* binding recognition of phospholipid-guanidinium interactions at the air/water interface. **J.F. Neal**, W. Zhao, A. Grooms, A.H. Flood, H.C. Allen

11:00 ENVR 378. Urea functionalization of biochar activated by ultrasound: An efficient strategy for heavy metal adsorption. **B. Sajjadi**, J. Broome, W.W. Chen

11:20 ENVR 379. Developing quantitative modeling framework for better understanding interconnected food-energy-water systems. **Y. Yao**, R. Huang

11:40 ENVR 380. Harmattan and the food,energy and water nexus. **C. Unegbu**

Section B
Ernest N. Morial Convention Center
Room 347

Current State of Environmental Contamination Research: Theory & Experiment
Cosponsored by CEI
G. Jenness, H. McAlexander, *Organizers*
S. Ahuja, M.K. Shukla, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 381. Three dimensional structures of human nicotinic acetylcholine receptor β4b2 constructed through homology modelling and molecular dynamics simulation. **H. Hong**

8:30 ENVR 382. Development of chitosan wrapped CNT based 3D nanoporus membrane for separation and inactivation of *Rotavirus* and *Shigella* waterborne pathogens. **P.C. Ray**

8:55 ENVR 383. Historical trends of polychlorinated biphenyls in Chesapeake Bay fish and the influence of ongoing sources. **T. Needham**, U. Ghosh

9:20 Intermission.

9:35 ENVR 384. Degradation of short chain chlorinated paraffins (SCCPs) mediated by intact pumpkin and soybean seedlings. **Y. Li**, J. Liu, J.L. Schnoor, G. Jiang

10:00 ENVR 385. Can β-cyclodextrin attenuate the negative health effects of perfluorooctanoic acid? **M.J. Weiss-Errico**, J. Miksovska, K.E. O'Shea

10:25 ENVR 386. Charactrization of nine haloacetaldehyde formation during chlorination of bromide-containing water. **M. Yuqin**, H. Yang, Y. Xie

10:50 Intermission.

11:05 ENVR 387. Formation of dioxins from 2-chlorophenol over fly ash: Role of Fe_2O_3. **X. Guan**, S.M. Lomnicki

11:30 ENVR 388. Kinetic of monochloramine reactions with nitrogenous compounds in aqueous solutions. **J. Wewers**, J. Gleason, K.P. Ishida, S.P. Mezyk

Section C
Ernest N. Morial Convention Center
Room 348

Innovative Chemical & Material Approaches for Sustainable Water Purification

Catalysis

Cosponsored by CEI
J. Choe, J. Liu, D. Shuai, Y. Wang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 389. Sustainable treatment of toxic 4,4′-thiodianiline in water using an enzyme. **D. Mukherjee**, K.E. Taylor, N. Biswas

8:55 ENVR 390. Advancing biocatalytic applications in drinking water: Column treatment of the disinfection byproduct chlorite. **J.M. Hutchison**, I. Kamalanathan, C.J. Werth, J. Zilles

9:15 ENVR 391. Expanding the catalyst toolbox – low-cost ruthenium catalysts for reduction of water contaminants. **X. Huo**, J. Liu, T.J. Strathmann

9:35 ENVR 392. Nitrogen-doped graphene supported Pd-based catalysts for water decontamination. **T. Ye**, D.P. Durkin, N. Banek, M.J. Wagner, D. Shuai

9:55 Intermission.

10:15 ENVR 393. Defluorination of branched per- and polyfluoroalkyl substances with cobalt complex catalysts. **J. Liu**, D. Van Hoomissen, X. Huo, X. Xiao, Y. Fang, C.P. Higgins, S. Vyas, T.J. Strathmann

10:35 ENVR 394. Cobalt catalyzed reduction of perfluoroalkyl substances: Reactions and mechanisms. **D.J. Van Hoomissen**, J. Liu, T.J. Strathmann, S. Vyas

10:55 ENVR 395. Catalytic destruction of oxyanions by bimetallic noble metal-based materials. **X. Min**, Y. Wang

11:15 ENVR 396. Biocatalytic membranes prepared by inkjet printing functionalized yeast cells onto microfiltration substrates. Y. Chen, P. Gao, M. Summe, W.A. Phillip, **N. Wei**

11:35 ENVR 397. Investigation of nanostructured MoS_2 as an earth abundant catalyst for nitrite hydrogenation. **R. Marks**, K. Doudrick

11:55 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 349

Advances & Applications in Water Sensing Technologies for Drinking Water & Agri-Tech Research

M.E. Romero-Gonzalez, P.L. Schorr, W. Zhang, *Organizers, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 398. Could advances in water sensing technologies with "near real time' monitors highlight chemical, biological and physical kinetics of complex river systems? **P.L. Schorr**, W. Zhang

8:40 ENVR 399. Development of autonomous sensing platform for in-situ nutrient analysis in marine and fresh waters. **M. McCaul**, D. Diamond

9:00 ENVR 400. Array sensing for trace detection of metal cations using optical spectroscopic techniques. **M. Ihde**, J. Tropp, A. Mallet, J.D. Azoulay, K.J. Wallace, M. Bonizzoni

9:20 ENVR 401. Assessing spatial or temporal variability in pCO_2 dynamics of estuarine and freshwater ecosystems: Case studies from North Carolina and China demonstrate trade-offs. **B.R. Van Dam**, J. Crosswell, H. Paerl

9:40 ENVR 402. Hourly changes in factors affecting algal blooms in an urban river with wastewater reuse and drinking water intakes can be evaluated using a neural network. **P.L. Schorr**, K. Li

10:00 Intermission.

10:15 ENVR 403. Detection of polycyclic aromatic hydrocarbons by chemical fingerprinting. N. White, J. Tropp, J.D. Azoulay, **M. Bonizzoni**

10:35 ENVR 404. Detection of nanoparticles on plant tissues using sp-ICP-MS. **Y. Huang**

10:55 ENVR 405. Charge-assembled fluorescent gold microcapsules with enhanced chromium(VI) sensitivity. **Y. Yin**, C. Coonrod, K. Heck, M.S. Wong

11:15 ENVR 406. Highly Sensitive electrically-receptive thermally-responsive analytical biosensor chip for rapid detection of *Bacterial cells*. **S.K. Misra**, M.S. Khan, Z. Wang, K. Dighe, A.S. Schwartz-Duval, D. Pan

11:35 ENVR 407. Withdrawn

Section E
Ernest N. Morial Convention Center
Room 350

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

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T. Anumol, R. Marfil-Vega, T.M. Young, C. Zwiener, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 408. Quantification and suspect-screening of hydrophobic and hydrophilic quaternary ammonium compounds in water samples by LC-HRAM-MS/MS. **S.G. Pati**, X. Ming, W. Arnold

8:30 ENVR 409. Identification of sources, occurrence and fate of the fungicide carbendazim in water. S. Merel, S. Benzing, J. Yanez Heras, **C. Zwiener**

8:55 ENVR 410. High resolution-MS uncovers new chemicals of concern in drinking water: Impacts of hydraulic fracturing and wastewater reuse. **S.D. Richardson**, H.K. Liberatore, K.H. Cochran, C. Montagner, D. Westerman, M.J. Plewa, L.H. Cizmas, J.M. Vanbriesen, D.D. Dionysiou, D. Schlenk, K. Loftin, T. Anumol

9:20 ENVR 411. Workflows utilizing SWATH and MRMHR acquisitions for microcystins in drinking water. **K. Hyland**

9:45 Intermission.

10:10 ENVR 412. High resolution mass spectrometry screening of urban stormwater for identification of novel contaminants and their sources. **E.P. Kolodziej**, K. Peter, B. Du, C. Wu

10:35 ENVR 413. Withdrawn.

11:00 ENVR 414. Withdrawn.

11:25 ENVR 415. Broad-scope LC and GC-HRMS screening for organic contaminants in wastewater at the sub-sewershed scale. M. Hattaway, J. Teerlink, C. Alaimo, T. Anmol, **T.M. Young**

11:50 Discussion.

Section F
Ernest N. Morial Convention Center
Room 351

Approaches to Fill Data Gaps for Chemical Sources of Risk

C.I. Nicolas, *Organizer*
K. Philips, *Organizer, Presiding*
C.I. Nicolas, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR 416. US EPA CompTox Chemistry Dashboard as a source of data to fill data gaps for chemical sources of risk. **A.J. Williams**, C. Grulke, K. Mansouri, K. Dionisio, K. Phillips, G. Patlewicz, I. Shah, K. Isaacs, J. Wambaugh, A. Richard, R. Judson

8:30 ENVR 417. Implementation of a web-based workflow for evaluation of chemical risks in the Superfund program. **A. Frame**, A.J. Williams, R. Judson, R. Sams, C. Grulke, I. Shah, G. Patlewicz, J. Lambert, S. Wesselkamper, S. Foster, K. Raffaele

8:50 ENVR 418. NICEATM's ICE Tool: An integrated chemical environment to support novel toxicological approaches. **N. Kleinstreuer**, S. Bell, J. Phillips, X. Chang, Q. Zang, D. Allen, W. Casey

9:10 ENVR 419. Rapid and accurate quantum chemical physicochemical property computational estimates for under-characterized compounds. **W.A. Alexander**

9:30 ENVR 420. Chemical toxicity prediction for major classes of industrial chemicals: Is it possible to develop universal models covering cosmetics, drugs, and pesticides? V.M. Alves, **E. Muratov**, A. Zakharov, N. Muratov, C.H. Andrade, A. Tropsha **9:50** Intermission.

10:05 ENVR 421. Case studies in characterising metabolic similarity in read-across through the use of *In vitro*, *In silico* and analytical data. **G. Patlewicz**, L. Lizarraga, E. Owens, J. Lambert, S. Wesselkamper, Q.J. Zhao, B. Hawkins, J. Dean, A.J. Williams, I. Shah, K.A. Favela, A. Yau, J. Bonzo, L.R. Moody, R. Thomas, J. Wambaugh

10:30 ENVR 422. Virtual screening of chemicals for endocrine disrupting activity: Case studies of the estrogen and androgen receptors. **K. Mansouri**, N. Kleinstreuer, C. Grulke, A. Richard, I. Shah, A.J. Williams, R. Judson

10:50 ENVR 423. Application of multiple *in silico* methods for evaluating potential liver toxicity of phytochemicals. **Y. Liu**

11:10 ENVR 424. Computational approaches to evaluate mode of action interactions and uncertainties: Thiocyanate as case study. **M. Willemin**, L. Jung, A. Lumen

11:30 ENVR 425. Rapid speciation and determination of vanadium compounds by ion-pair reversed-phase ultra-high-performance liquid chromatography inductively coupled plasma-sector field mass spectrometry: *In vitro* speciation models. **J.M. Harrington**, L.G. Haines, A.S. Essader, K.E. Levine, R.A. Fernando, V.G. Robinson, S. Waidyanatha

11:50 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 342

Advances in Understanding of Sorptive & Reactive Properties of Pyrogenic Carbonaceous Matter (PCM) in the Environment

W. Mitch, W. Xu, *Organizers*
J.J. Pignatello, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 ENVR 426. Factors controlling the adsorption of ionizable compounds to activated carbon. **D. Knappe**, L. Dudley, A. Rossner, M. Sun

8:55 ENVR 427. Thermodynamics of attachment: Enthalpy and free energy of adsorption of neutral and ionic micropollutants on biosolids-derived biochar. **Y. Tong**, P.J. McNamara, S.L. Singer, B. Mayer

9:15 ENVR 428. Elimination of a potentially hazardous, flame retardant chemical consisting of an organophosphorus moiety from water using biochar as an adsorbent. **A. Saha**, S.R. Akech

9:35 ENVR 429. Development of improved biochars through alkaline pretreatment and metal catalysis for the removal of organic micropollutants in source water protection scenarios. **M. Bentley**, R.S. Summers

9:55 ENVR 430. Sorption of hydrophobic organic compounds to dissolved black carbon and impact of its release on sorption properties of bulk black carbon. H. Fu, B. Wang, X. Qu, H. Li, W. Zhang, **D. Zhu**

10:15 Intermission.

10:30 ENVR 431. High temperature co-pyrolysis/thermal air activation modifies biochar porosity and enhances capacity for uptake of herbicides from surface water. **J. Kearns**, K. Shimabuku, D. Knappe, R.S. Summers

10:50 ENVR 432. Biomass-converted graphene-like material for the ultra-high adsorption of organic pollutants. **X. Xiao**, B. Chen, L. Zhu, J.L. Schnoor

11:10 ENVR 433. Evaluating biochar in sustainable stormwater treatment of heavy metals. **S. Burch**, J.A. Nason

11:30 ENVR 434. Selective recovery of thorium by wrinkled mesoporous carbon. Z. Wang, **K.J. Balkus**

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Kinetics

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Sponsored by GEOC, Cosponsored by ENVR

Lignin: From Fundamentals to New Materials & Applications

Nanoscaled Materials from Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Confinement: Clay Mineral Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

R&D in the Chemical Catalysis for Bioenergy Consortium
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Catalysis & Surface Science Science Applied to the Destruction of Threat Agents

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 346

Novel Concepts in the Role of Chemistry in the Food, Energy & Water Nexus
Cosponsored by MPPG
S. Ahuja, D.D. Dionysiou, *Organizers*
S. Chae, I. Chowdhury, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 435. Chlorotyrosines versus volatile byproducts from disinfection during washing of lettuce and spinach. **W. Mitch**, Y. Komaki, A. Simpson

2:05 ENVR 436. Attachment of foodborne microbes to spinach leaf surfaces: The role of solution chemistry and growth conditions. **H. Mayton**, I. Marcus, S.L. Walker

2:25 ENVR 437. Assessing risks from pharmaceuticals and transformation products in urine-derived fertilizers. **W. Tarpeh**, D.S. Aga, K. Wigginton, N. Love

2:45 ENVR 438. Role of ferrate technology in the food, energy, and water nexus. **V.K. Sharma**

3:05 ENVR 439. Educating the community on the interconnectedness of energy, food and water sustainability as we seek to reduce exposure to environmental toxics. **R.C. Wingfield**, K. Jackson, V. Watson

3:25 Intermission.

3:40 ENVR 440. Elucidating nanoparticle-plant leaf interactions, uptake, and mobility for designing highly efficient foliar-applied agrochemicals. **A. Avellan**, J. Yun, E. Spielman-Sun, G. Lowry

4:00 ENVR 441. Toward improving agrochemical efficiency: Impact of Cu-based nanoparticle solubility on metal uptake, speciation, translocation, and distribution in *Triticum aestivum* (wheat). **E. Spielman-Sun**, E. Lombi, E. Donner, B. Etschmann, D. Howard, G. Lowry

4:20 ENVR 442. Reduction of excess biological sludge in tannery effluent treatment. **V. Sodhi**, A. Bansal, **M.K. Jha**

4:40 ENVR 443. Alberta oil sands extraction and tailings ponds emissions: Predicting the fate of thousands of oil hydrocarbon compounds simultaneously. B. Drollette, **D.L. Plata**

Section B
Ernest N. Morial Convention Center
Room 347

Current State of Environmental Contamination Research: Theory & Experiment
Cosponsored by CEI
S. Ahuja, G. Jenness, *Organizers*
H. McAlexander, M.K. Shukla, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 444. Energetics and vibrational signatures of argyrophilic interactions involving high energy density materials. **G.S. Tschumper**

2:00 ENVR 445. Kinetic Monte Carlo models to study nucleation and evolution of metal/metal oxide nanoparticles grown via aerosol route. **D. Mukherjee**

2:25 ENVR 446. Adsorption of some

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munitions compounds on silica surfaces: A density functional theory investigation. **R.K. Chouhan**, G. Subramanian, M.K. Shukla

2:50 Intermission.

3:05 ENVR 447. Trajectory-based models and remote sensing for biomass burning assessment in Bangladesh. **F. Emami**, P. Hopke, A. Ommi

3:30 ENVR 448. Development of accurate force-fields for water clusters with acidic defects. **R. Kumar**, C. Bresnahan

3:55 ENVR 449. Synergy between palladium and indium during heterogeneously catalyzed nitrate degradation. S. Kasiraju, S. Guo, K. Heck, H. Qian, Z. Zhao, J.T. Miller, M.S. Wong, **L. Grabow**

4:20 Intermission.

4:35 ENVR 450. Theoretical investigation of ground and excited electronic states of the water splitting catalytic cycle facilitated by MoO^{+}. **E. Miliordos**

5:00 ENVR 451. Mathematical modeling tools for characterizing vapor intrusion: Challenges for gaining acceptance. **E. Suuberg**, J. Ström, A. Oliveira

Section C
Ernest N. Morial Convention Center
Room 348

Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery
Cosponsored by CEI
X. Mao, Y. Men, W. Zhuang, *Organizers*
C.M. Sales, S. Yi, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 452. Examining nutrient uptake and transformation within photosynthetic microbial communities using a high density bioreactor. **J. Price**, C.M. Sales

1:55 ENVR 453. Integrated meta-omics approach reveals synergistic interactions in a bisphenol- A-degrading microbial community. **K. Yu**, S. Yi, B. Li, L. Alvarez-Cohen, T. Zhang

2:15 ENVR 454. Reconstruction of cellulose-to-methane trophic chain from metagenomics and metatranscriptomics. Y. Jia, **P.K. Lee**

2:45 ENVR 455. Global wastewater microbiome: Diversity and biogeography. **J. Zhou**, X. Wen, T. Curtis, Q. He, D. Ning, Y. Yang, L. Wu, B. Zhang, F. Ling

3:15 Intermission.

3:30 ENVR 456. Genome-resolved metagenomics to assess the long-term impact of disinfection on the drinking water microbiome. **A.J. Pinto**

4:00 ENVR 457. Characterization of the microbial community driving on-site wastewater treatment in nitrogen removing biofilters (NRBs). **K. Langlois**, J.L. Collier, N. Volkenborn, M. Graffam

4:20 ENVR 458. Impact of material electrical conductivity on the microbial community structure in anaerobic digesters. **Q. Cheng**, F.L. de los Reyes, D.F. Call

4:40 ENVR 459. Microbial community structure and electrochemical activity during the formation of successful versus failed electroactive biofilms. **J. Ortiz Medina**, D.F. Call

Section D
Ernest N. Morial Convention Center
Room 349

Water Use Optimization: Water Quality, Reuse & Treatment

Water Reuse & Water Quality

S. Bushart, Y. Jun, K. Pagilla, N. Rao, Y. Yang, *Organizers, Presiding*

1:30 ENVR 460. Connecting recycled water to spreading basins for combined operation and greater water supply resiliency. J. Bradshaw, N. Ashoori, M. Osorio Gonzalez, T. Schmitt, **R.G. Luthy**

2:00 ENVR 461. Water reuse project at University of Nevada-Reno: Addressing human healthiImpacts from emerging contaminants in reclaimed water to enhance its use for urban and peri-urban agriculture. **K. Pagilla**, P. Verburg, D. Hanigan, Y. Yang

2:20 ENVR 462. Effects of oxyanions on arsenic mobilization from arsenopyrite during managed aquifer recharge. **X. Wu**, S. Burnell, C. Neil, D. Kim, H. Jung, Y. Jun

2:40 ENVR 463. Disinfection byproducts removal during water reuse using natural solar photo-fenton process. **I. Abusallout**, G. Hua

3:00 ENVR 464. Optimized pilot-scale recovery of abandoned mine drainage for reuse in hydraulic fracturing using nanofiltration membranes. **S. Wadekar**, T. Hayes, D. Mittal, R.D. Vidic

3:20 ENVR 465. Withdrawn.

3:40 Intermission.

3:50 ENVR 466. Electrodialysis metathesis for desalination of geothermal waters and recovery of rare earth elements: Role of pH and solubility. L.M. Camacho, **M. Shafiq**

4:10 ENVR 467. Experimental investigations for efficient removal of ultrafine coal particles from effluent streams: Bench and pilot-scale studies. A. Bhagavatula, V. Rajagopalan, **B. Duncan**, P. Vimalchand, M. Nelson

4:30 ENVR 468. Sensitivity of watershed delineation and modeled hydrology and water quality to topographic characteristics of watersheds. **Z. Duan**, J. Diaz-Ramirez, J. Martin, S. Xie, Z. Chen, J. Wang

4:50 ENVR 469. Determination of perchlorate by US EPA Method 332.0 using a compact ion chromatography system coupled with mass spectrometry (IC-MS). **B. Huang**, J. Rohrer

5:10 ENVR 470. Development of a U.S. EPA method for the analysis of nonylphenol in drinking water by solid phase extraction and LC/MS/MS. **D.R. Tettenhorst**, J.A. Shoemaker

Section E
Ernest N. Morial Convention Center
Room 350

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

T. Anumol, R. Marfil-Vega, T.M. Young, C. Zwiener, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 471. Quality control, validation and strategies for statistical analysis in chemometric approaches using high-resolution MS in environmental and waste waters. **D. Cuthbertson**

2:00 ENVR 472. Improving confidence in environmental contaminant identification with highly curated databases and accurate mass MS/MS libraries. **R. Garnica**, E.E. Rennie, T. Anmol, S. Xu, J. Zweigenbaum, M. Miladi

2:25 ENVR 473. Tracing the biotransformation of PAHs in contaminated soil using stable isotope-assisted metabolomics. **Z. Tian**, J. Vila, M. Yu, W. Bodnar, M. Aitken

2:50 ENVR 474. Target, suspect and non-target screening of dioxin-like compounds in environmental samples using a sensitive high-resolution time-of-flight mass spectrometer. **P. Haglund**, N. Eno, S. Nieto

3:15 Intermission.

3:40 ENVR 475. Molecular-level insights into environmental organic contaminants by high resolution fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry. **R.P. Rodgers**, S. Rowland, H. Chen, A.M. McKenna, P. Zito, Y. Corilo

4:05 ENVR 476. Characterization of naphthenic acids and other dissolved organics in natural water from the Athabasca Oil Sands Regions, Canada by using ultra-high resolution Orbitrap mass spetrometry. **C. Sun**, J. Martin, W. Shotyk

4:30 ENVR 477. Analysis of halogenated combustion byproducts in soot on firefighter protection equipment and skin after structural fires. **C. Hoppe-Jones**, S. Beitel, L. Flahr, S.A. Snyder

4:55 ENVR 478. Transformation of dissolved organic matter in engineered ultraviolet (UV) photolysis and UV-based advanced oxidation processes. **D. Minakata**, L. Varanasi, M. Khaksari, L.R. Mazzoleni

5:20 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 351

Contaminants in Water Sources Impacted by FEW Systems: Emerging Challenges & Opportunities

D.M. Cwiertny, *Organizer*
C.L. Just, G.H. LeFevre, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 479. Environmental photochemistry of dichloroacetamide herbicide safeners. A.E. Kral, M.E. McFadden, G.H. LeFevre, J.D. Sivey, **D.M. Cwiertny**

1:55 ENVR 480. Adsorption of double-stranded RNA (dsRNA) at solid-water interfaces: Implications for the environmental fate of dsRNA biopesticides from RNA interference (RNAi) agricultural biotechnology. **K. Parker**, M. Sander

2:15 ENVR 481. Impact on surface water quality due to the enhanced solubility of organochlorine pesticides following an ethanol-blend fuel spill. **M. Otero-Diaz**, B. Woo, N. Bhattacharyya, L. Ma, A. Demond

2:35 ENVR 482. Dichloramine reactivity with amino acids in wastewater. **E. Walker**, K.P. Ishida, S.P. Mezyk

2:55 ENVR 483. Transformation of neonicotinoid insecticides during disinfection under defacto water reuse. **G.H. LeFevre**, K. Klarich, D.M. Cwiertny

3:15 Intermission.

3:25 ENVR 484. Halogenation of agrochemicals and related compounds in waters disinfected with free chlorine: Competition between rates of chlorination and bromination. **J.D. Sivey**, M.A. Broadwater, T.L. Swanson, R.P. Dias, A.L. Roberts

3:45 ENVR 485. Sorption of neonicotinoid insecticides to granular activated carbon during drinking water treatment. **D. Webb**, K.L. Klarich, G.H. LeFevre, D.M. Cwiertny

4:05 ENVR 486. Combining HRMS-based suspect screening and statistical analysis to assess contaminants of emerging concern in a wastewater-impacted urban lake. **S. Wang**, T. Zeng

4:25 ENVR 487. Influence of climate change on subsurface atrazine degradation and transport. **S. Bartelt-Hunt**, R. Barrios, O. Gaonkar, X. Li, D.D. Snow, Y. Li

4:45 ENVR 488. Water quality as an additional factor for the energy-water nexus: Distribution of contaminants in water impacted by fossil fuels activities. **A. Vengosh**

5:05 ENVR 489. Effect of dissolved organic matter on the photochemical transformation of trace organic contaminants in wastewater: The role of singlet oxygen. **L. Ma**, H. Thi Hong Vo, R. Arnold, A.E. Saez

5:25 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 342

Advances in Understanding of Sorptive & Reactive Properties of Pyrogenic Carbonaceous Matter (PCM) in the Environment

J.J. Pignatello, W. Xu, *Organizers*
W. Mitch, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR 490. Surface-promoted hydrolysis of 2,4,6-trinitrotoluene and 2,4-dinitroanisole on pyrogenic carbonaceous matter. **K. Ding**, C. Byrnes, A.M. Grannas, W. Xu

1:55 ENVR 491. Inherent reactivity of chars from model feedstocks, lignin and cellulose: Persistent free radicals, reactive oxygen species, and non-radical direct reacting sites. **J.J. Pignatello**, J. Yang, B. Pan, B. Xing

2:30 ENVR 492. Redox properties of water-extractable dissolved organic matter (DOM) from plant biomass –

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derived black carbon (biochar). **W. Xu**, N. Walpen, M. Keiluweit, M. Kleber, M. Sander

2:50 ENVR 493. Photoactivity of dissolved black carbon in natural aquatic systems. H. Fu, **X. Qu**, D. Zhu

3:10 Intermission.

3:25 ENVR 494. Capture and dehalogenation of fipronil using a semi-passive black carbon-based electrode. **W. Mitch**, Y. Li

3:45 ENVR 495. Desalination with capacitive deionization under various operating conditions and electrode configuration using Carbon fiber/paper electrodes. **M. Ahmed**, S. Tewari

4:05 ENVR 496. Abiotic reduction of nitrobenzene with sulfide catalyzed by carbon nanotubes in aqueous solutions: Effect of surface modification and parameter optimization. **H. Zhao**

4:25 ENVR 497. Probe the surface reactivity of pyrogenic carbonaceous materials using conjugated microporous polymers. **Z. Li**, J. Mao, W. Xu

Unconventional Catalysis Targeting Stable Molecules
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Sponsored by GEOC, Cosponsored by ENVR

Lignin: From Fundamentals to New Materials & Applications

Carbon Fibers & Chemicals from Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Carbonates, Phosphates & Rare Earth Elements

Sponsored by GEOC, Cosponsored by ENVR and INOR

Forensic Geochemistry
Sponsored by GEOC, Cosponsored by ENVR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

R&D in the Chemical Catalysis for Bioenergy Consortium
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Photocatalytic Approaches

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

WEDNESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

T. Anumol, R. Marfil-Vega, T.M. Young, C. Zwiener, *Organizers*

6:00–8:00

ENVR 498. High resolution mass spectrometry analysis of biomass burning organic aerosol composition from different wood fuels and combustion conditions. **K. Nguyen**, H. Bayat, M. Hengel, T.B. Nguyen

Section A
Ernest N. Morial Convention Center
Hall D

Advances in Understanding of Sorptive & Reactive Properties of Pyrogenic Carbonaceous Matter (PCM) in the Environment

W. Mitch, J.J. Pignatello, W. Xu, *Organizers*

6:00–8:00

ENVR 499. Adsorption characteristics of benzalkonium chloride (BAC) by activated carbon. **W. Choi**, T. Kim, K. Zoh

ENVR 500. Characterization of biochars structure and the applications as a sorbent. **X. Xiao**, B. Chen

ENVR 501. Highly effective catalytic peroxymonosulfate activation on mesoporous carbon nitride for o-phenylphenol degradation. J. Hou, **S. Zheng**, D. Zhu

Section A
Ernest N. Morial Convention Center
Hall D

Agro-Environmental & Energy Applications of Biochar/Hydrochar

N.D. Berge, C. Jeong, K. Ro, *Organizers*

6:00–8:00

ENVR 502. Chromium ion removal from aqueous media by aluminum and magnesium impregnated biochar. **A. Herath**, C. Layne, G. Burk, T. MIsna

ENVR 503. Graphene coated pine wood biochar from slow pyrolysis to decontaminate copper from aqueous solutions. **H. Samaraweera**, T. MIsna

ENVR 504. Pine wood biochar to decontaminate Cu(II) from aqueous solutions. **A. Hanson**, H. Samaraweera, T. MIsna

ENVR 505. Removal of lead from aqueous systems by potassium hydroxide activated biochar. **C. Layne**, A. Herath, T. MIsna

ENVR 506. Recycling phosphate with MgO decorated magnetic biochar composite and its potential use as fertilizer. **B. Zhou**, R. Li, J.J. Wang

ENVR 507. Nitrogen sorption by biochars derived from different feedstocks and at different pyrolysis temperatures: Affecting factors and mechanisms. **S. Li**, V. Barreto, R. Li, G. Chen, Y.P. Hsieh

ENVR 508. Preparation and re-activation of nitrogen-doped magnetic biochar by molten salt method: Relevant performance for organic pesticides removal. **S. Dai**, Y. Zhao

ENVR 509. Adsorption mechanism of Cu(II) on crop-residue char. **S. Wang**, I. Liao, R. Chang

ENVR 510. Effects of poultry-manure biochars on the soil phosphorus availability to rice plant. M. Soesanto, Y. Hashimoto, M. Cheng, **S. Wang**

Section A
Ernest N. Morial Convention Center
Hall D

Antibiotics & Antimicrobial Resistance: Developing Solutions to Address the Connectivity Between Air, Food, Water & Soil

D.S. Aga, X. Li, A. Pruden, P.J. Vikesland, *Organizers*

6:00–8:00

ENVR 511. Tylosin sorption to diatomaceous earth: Investigation of physical processes of tylosin in natural systems and development of mitigation methods. **B. Stromer**, B. Woodbury, C. Williams

ENVR 512. Antimicrobial susceptibility, stress responses, and hormesis in *Pseudomonas fluorescens* as metrics for assessing impacts of antibiotics in the environment. **E.R. Hain**, H. Adejumo, L.M. Blaney

ENVR 513. Superspreader phage-mediated dissemination of antibiotic resistance gene-containing plasmids in wastewater disinfection processes. **M. Gnegy**, A. Pruden, P.J. Vikesland, K. Wigginton

ENVR 514. Detection and evaluation of antibiotics in seven wastewater treatment plants in Southwest Illinois. **Q. Zhang**, C. Donald, J. Rhomberg, K. Tucker

ENVR 515. Large-scale modeling of the antibiotic resistance: A hydrological perspective. **M. Thilakarathne**, V. Sridhar

ENVR 516. Lessons learned on the fate of ARG in end-of-pipe treatment systems for combined sewer overflows. A. Eramo, H. Delos Reyes, W. Morales Medina, **N. Fahrenfeld**

Section A
Ernest N. Morial Convention Center
Hall D

Approaches to Fill Data Gaps for Chemical Sources of Risk

C.I. Nicolas, K. Philips, *Organizers*

6:00–8:00

ENVR 517. Effect of toxicity, distribution and metabolism for co-occurring exposure to microplastics and the chiral antidepressant venlafaxine in loach (*M.anguillicaudatus*). **H. Qu**, R. Ma, B. Wang

ENVR 518. OpenRiskNet, an open e-infrastructure to support data sharing, knowledge integration, *in silico* analysis and modelling in risk assessment. **N. Oki**, T. Exner, S. Kramer, C. Notredame, D. Jennen, G. Gkoutos, H. Sarimveis, M. Jacobs, O. Spjuth, T. Dudgeon, F. Bois, P. Jennings, B. Hardy

Section A
Ernest N. Morial Convention Center
Hall D

Aquatic Photochemistry

W. Arnold, K.P. McNeill, S.G. Pati, *Organizers*

6:00–8:00

ENVR 519. Photochemistry of atmospheric carbonyl reaction products. **M.M. Galloway**, J.M. Ackendorf, M.B. Sebold, D.N. Grace, R. Holappa

ENVR 520. Photochemical oxidation reduces the efficacy of aerial dispersants applied in response to oil spills. C.P. Ward, **C.J. Armstrong**, C. Reddy

ENVR 521. Withdrawn.

ENVR 522. Apparent quantum yields of singlet oxygen and photochemical oxygen consumption for crude oils. **C.P. Ward**, C. Reddy, **C.M. Sharpless**

ENVR 523. Photodegradation of sulfathiazole: Kinetics, photo-induced structural rearrangement, and photoproducts antimicrobial activities. **X. Niu**, J. Croue, J. Glady-Croue

ENVR 524. Comparative study of the photochemical fate of ebselen and its carbon analog during direct and indirect photolysis. **M. Hopanna**, S. Steinly, L.M. Blaney

ENVR 525. Photodegradation of o-phthalic acid and the effects of nitrite and nitrate. **X. Lu**, Y. Zuo

ENVR 526. Analysis of the characterization and toxicity of ultraviolet filter chemical (UVFC) octyl dimethyl para-aminobenzoic acid (OD-PABA) photoproducts. **L. O'Connor**, J. Maung, L. MacManus-Spencer, M.G. Paulick

ENVR 527. Photolysis and cellular toxicity of the organic ultraviolet filter chemical 2-ethylhexyl-4-(dimethylamino)benzoate (OD-PABA) and its photoproducts. **J. Maung**, L. O'Connor, M.G. Paulick, L. MacManus-Spencer

ENVR 528. Effects of natural water matrix on the aquatic photodegradation of 17β-ethynylestradiol (EE2). **Y. Zuo**, F. Albalawi

ENVR 529. Effects of halide ions on photodegradation of sulfonamide antibiotics: Formation of halogenated intermediates. **X. Qiao**

ENVR 530. Photodegradation of methylparaben in aquatic environment: Kinetics and reaction mechanisms. **Y. Deng**

ENVR 531. Sorption of model micropollutant to polyethylene film after UV exposure. **F.E. Murphy**, M.A. Maurer-Jones

ENVR 532. Effects of precursors on the photocatalytic activities of graphitic carbon nitride in hexavalent chromium

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reduction and rhodamine B degradation under visible light irradiation. **C. Chuaicham**, K. Sasaki

ENVR 533. Characterizing the effects of sethoxydim on the photosynthetic activity and biochemical composition of *Chlorella vulgaris*. **A. Smythers**, A. Garmany, N. Perry, P.E. Adkins, E. Higginbotham, D. Kolling

ENVR 534. Inactivation kinetics of *E. coli* and MS2 coliphage by photogenerated singlet oxygen. **T. Kim**, H. Kim, H. Kim, J. Seo, J. Lee, C. Lee

Section A
Ernest N. Morial Convention Center Hall D

Chemistry of Drinking Water Distribution Systems & Infrastructure

D. Giammar, Y. Hu, H. Liu, *Organizers*

6:00–8:00

ENVR 535. Montebello water filtration plant-I in Baltimore: Chemistry's contribution to public health. **B. Salazar**, **P.J. Smith**, **R. Nuss**

ENVR 536. Snapshot of lead and copper in Iowa drinking water. **A. Grant**, D. Latta, S. Dai, D.M. Cwiertny, M. Scherer

Section A
Ernest N. Morial Convention Center Hall D

Contaminants in Water Sources Impacted by FEW Systems: Emerging Challenges & Opportunities

D.M. Cwiertny, C.L. Just, G.H. LeFevre, *Organizers*

6:00–8:00

ENVR 537. Accumulation of copper in sediments of lakes treated with copper-based pesticides. **M. Albalawi**, M.J. Beazley

ENVR 538. Bioaugmentation and phytoremediation of 1,4-dioxane in simulated groundwater. **R. Simmer**, J.L. Schnoor

ENVR 539. Role of abiotic and biotic denitrification in agricultural soils. **O.B. Felber**, D. Latta, M. Scherer, C.L. Just

ENVR 540. Degradation comparison of pentachlorophenol (PCP) versus pentachloroanisole (PCA) using zero-valent magnesium/graphite (ZVMg/C) in an acidified ethanol. **A. Garbou**, C. Clausen, C. Yestrebsky

ENVR 541. Meta-analysis of nanoparticle toxicity: Determining effect of units and identifying future directions. **R.M. Wheeler**, S. Lower

ENVR 542. Removal of perchlorate from water: Environmental chemistry. **A. Plank**, A. Mueller

ENVR 543. Community usage of illicit drugs in Western Kentucky, USA. **K.S. Foppe**, B. Subedi

ENVR 544. Suppression mechanism of anionic pollutants released from fly ash by Ca additives. S. Nakama, Q. Tian, B. Guo, N. Pahlevi, Z. Hu, **K. Sasaki**

ENVR 545. Determination of chemicals of emerging concern in plant tissues using isotope-dilution microwave-assisted extraction and LCMSMS. **O. Quinones**, B. Vanderford, E. Dickenson

ENVR 546. Transformation of pharmaceuticals during dielectric barrier discharge plasma jet treatment in synthetic urine. **E. Rodriguez**, W. Tarpeh, H. Clack, K. Wigginton, N. Love

ENVR 547. Occurrence, fate, and composition of N-nitrosamines and their precursors in wastewater. **C. Pu**, T. Zeng

ENVR 548. Reductive dechlorination of 1,2-dichloroproane by ZVI with vitamin B12. **N. Lapeyrouse**, G.J. Booth, C. Yestrebsky

ENVR 549. Levels and ecological risks of selected endocrine disrupting compounds (EDCs) in the urban surface water of New Calabar River, Port Harcourt City, Nigeria. **E. Inam**, **N.O. Offiong**, E.D. Essien, I. Nwoke

Section A
Ernest N. Morial Convention Center Hall D

Current State of Environmental Contamination Research: Theory & Experiment

S. Ahuja, G. Jenness, H. McAlexander, M.K. Shukla, *Organizers*

6:00–8:00

ENVR 550. N,N-Dimethyl-p-nitrosoaniline and potassium linoleate hydroperoxide as spin traps in process of hydroxyl radicals formation during chloride-free electrolysis of contaminated water. **N. Barashkov**, T. Sakhno, I. Irgibayeva, A. Aldongarov, A. Mantel

ENVR 551. Investigation of the presence of heavy metals in water and fish from bon accord dam in northern Tshwane, South Africa. **O.O. Oyewole**

ENVR 552. Adsorption of amlodipine and carbamazepine at the air-aqueous interface and onto colloidal surfaces mimicking natural organic matter. **T.A. Williams**, M. Subir

ENVR 553. Irradiation of aqueous solutions of NTO, NQ and DNAN at UV wavelengths. **J. Becher**, S. Beal, S. Taylor

ENVR 554.
Evaluating moss as biomonitors of atmospheric heavy metals in Oregon. **A.J. Miller**, A.E. Shiel, B. McCune, S. Jovan, S. Kiel, T. Rosenstiel, J.L. Fry

ENVR 555. Inhalation bioaccessibility of trace metals in $PM_{2.5}$ from three megacities of China: Assessments by simulated lung fluid (SLF) and diffusive gradients in thin films (DGT). Z. Zhao, L. Jin, **X. Luo**, J. Luo, J. Xie, Y. Chen, H. Li, X. Li

ENVR 556. Optimization of free and protein bound microcystin detection in sediments and aquatic organisms. **M. Bolotaolo**, I. Gennity, Y. Bong, B. Puschner, S. Lesmeister, S. Teh

ENVR 557. Aquatic photochemical reaction of divalent mercury with 3-mercaptopropionic acid and its environmental implications. **L. Si**, P.A. Ariya

ENVR 558. Computational investigation on electronic structures and properties of 4,6-bis(nitroimino)-1,3,5-triazinan-2-one: An insensitive munition compound. **K. Pittman**, G.S. Tschumper, M.K. Shukla, H. McAlexander

ENVR 559. Developing a yeast biosensor for measuring phosphate in natural waters. **J. Praner**

Section A
Ernest N. Morial Convention Center Hall D

Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery

X. Mao, Y. Men, C.M. Sales, S. Yi, W. Zhuang, *Organizers*

6:00–8:00

ENVR 560. Nitrogen flows in an anaerobic ammonium oxidation (anammox) reactor. **J. Lawrence**, L. Zhou, R. Keren, J. Banfield, C. Yu, L. Alvarez-Cohen

ENVR 561. Characterizing the potential of waste aerobic granular sludge as an ion-selective seed material for phosphorus recovery from nutrient rich wastewater. **D.B. Kitt**, R.D. Cusick

ENVR 562. Effects of transient hydrologic regimes upon nitrous oxide reduction in denitrifying bioreactors. **P.M. McGuire**, L. Falk, M.C. Reid

ENVR 563. Impact of legacy nitrogen in conventional septic system on nitrogen removal for onsite wastewater treatment. **Z. Maleki Shahraki**, X. Mao, S. Waugh, H. Walker

ENVR 564. Fabrication of cationic cellulose from natural bioresources for waste activated sludge dewatering treatment. **X. Huang**, P. Hadi, B.S. Hsiao

Section A
Ernest N. Morial Convention Center Hall D

Environmental Chemistry Undergraduate Education in the Classroom, Laboratory & Beyond

M. Berger, L.A. Welch, *Organizers*

6:00–8:00

ENVR 565. Impact of ocean acidification on the composition of marine shells. **M. Lopez**, **M. Flores**, P.R. Calvo, J. Del Pilar

ENVR 566. Introducing environmental chemistry topics into a first-year science writing course using narratives from geochemistry and evolutionary biology. **B.J. McFarland**

ENVR 567. Environmentalist in film. **F.M. Dunnivant**

Section A
Ernest N. Morial Convention Center Hall D

From Sewage to Sustainable Energy: Potential Pollution Issues from Production & Application Pathways

S. Chae, W. Giger, R. Kallenborn, A. Torrents, *Organizers*

6:00–8:00

ENVR 568. Withdrawn.

ENVR 569. Towards a Canadian national biosolids research agenda. **J.E. Loyo-Rosales**, L.H. McCarthy

Section A
Ernest N. Morial Convention Center Hall D

General Posters

S.O. Obare, *Organizer*
6:00–8:00

ENVR 570. Sustainable municipal wastewater treatment: Review of requirements and the urgency. **S. Chitikela**

ENVR 571. Measurement of nicotine emission rate in thirdhand smoke (THS). **M. Noguchi**, A. Yamasaki

ENVR 572. Naturally occurring radioactive materials in coals and coal ash in China. N. Lauer, **A. Vengosh**, S. Dai

ENVR 573. Determination of adsorbable organic halogen (AOX) in wastewater using combustion ion chromatography. **J. Hu**, J. Rohrer

ENVR 574. Quantifying rates of biological production to better understand the carbon cycle in the Canada basin. **B.Y. Ji**, R. Stanley

ENVR 575. Soil organic matter in native prairies and prairie restorations I: Organic carbon content. L.R. Morgan, B.M. Mullins, **J.S. McConnell**

ENVR 576. Soil organic matter in native prairies and prairie restorations II: Humic and fulvic acid fractions. S. Bomma, K. Pallempati, N. Voleti, **J.S. McConnell**

ENVR 577. Transformation of silver nanoparticles in surface waters. **C. Gagnon**, P. Turcotte, M. Pilote, F. Gagné, S. Smyth

ENVR 578. Withdrawn.

ENVR 579. Innovative materials management in open pit coal mines to reduce leachate conductivity. **S.R. Al-Abed**, P. Pinto, J. McKernan

ENVR 580. Potential role of dissolved molybdenum, iron, and vanadium in harmful algal blooms in Ohio lakes. **S.J. Israel**, S.A. Welch, W. Lyons

ENVR 581. Biological toxicity and FT-ICR MS characterization for photochemically degraded oil/water accommodated fractions as a function of wavelength exposure. **P.L. Bann**, S. Bilfulco, C. Brannon, L. Reid, B. Farran, W. Jeffrey, A.M. McKenna, C. Davis, **P.P. Benz**

ENVR 582. Biological toxicity of wavelength specific photochemically degraded water accommodated fractions. **C. Brannon**, L. Reid, P.L. Bann, W. Jeffrey, **P.P. Benz**

ENVR 583. Effects of burning and photochemical degradation of surrogate oil as a function of chemical characterization (determined by FT-ICR MS) and biological toxicity. **E. Post**, M. Seivert, W. Jeffrey, **P.P. Benz**

ENVR 584. Heavy metal remediation

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from aqueous solutions by new SIT materials. **E. Rush**, A.F. Callender, E.C. Lisic

ENVR 585. Radionuclides speciation in seawater. **C. Moulin**, C. Den auwer, M. Monfort, M. Beccia, B. Reeves, M. Maloubier

ENVR 586. Comparative approach to the understanding of Lake Trout contaminant dynamics in the Great Lakes. **J.J. Pagano**, A.J. Garner, T.M. Holsen

ENVR 587. Impact of energy in environmental pollusion. **T. Akinmusire**

ENVR 588. Preparation of super-hydrophobic and super-oleophilic porous alumina ceramics for oil/water separation. **X. Lv**, **T. Wang**

ENVR 589. Evidence for products of cross-reactions in organic films formed on sulfuric acid solutions at upper troposphere/lower stratosphere aerosol acidities. **T.E. Nelson**, J.H. Bui, E. Li, S. Perez-Montaño, A.L. Van Wyngarden

ENVR 590. Styrene oligomer contamination surround Japan in water and sand. **K. Koizumi**, Y. Kodera, T. Komoriya, K. Amemiya, K. Takatama, D.M. Karl, B. Kwon, S. Chung, **K. Saido**, T. Hiaki

ENVR 591. Distribution of soil phosphorus and nitrate in the Spring Lake watershed region of western Illinois. S. Nicioli, K.E. Ribordy, J. Boeckler, J.S. McConnell, **A.L. Hagen**

ENVR 592. Adsorption of BSA onto sodium saturated montmorillonite in the presence of monovalent, divalent, and trivalent cations. **A.L. Hagen**, M. Cash, J.S. McConnell

ENVR 593. Analysis of endocrine disrupting chemicals (EDCs) accumulation in Brown Planaria and its effects on regeneration. **R. AminiTabrizi**, R. Davis, B. Potter, K. Tucker

ENVR 594. Ionic/molecular sponge behavior of graphene oxide laminates. **Y. You**, X. Jin, R. Joshi

ENVR 595. Effects of exposure to light emitting diode (LED) using the model organism *Caenorhabditis elegans*. **F.H. Abdel-Rhman**, A. Aldawsari, K. Anthony, M.A. Saleh

ENVR 596. Oxidation of 3,5,6-trichloro-2-pyridinol by zero valent iron (ZVI) activated persulfate. **R.T. Mogharbel**, C. Yestrebsky

ENVR 597. Surfactant control of heterogeneous oxidation of atmospheric organic aerosol. **J. Faust**, J.P. Abbatt

ENVR 598. Sorption dynamics of cadmium and chromium (II) onto montmorillonite from mixed solvent systems. **M. Cash**, A.L. Hagen, J.S. McConnell

ENVR 599. Soil organic matter in native prairies and prairie restorations III: Structural studies of humic acids with carbon-13 NMR spectroscopy. A. Poladi, J.S. McConnell, **M. Cash**

ENVR 600. Removal of heavy metals in metal plating wastewater by powdered activated carbon (PAC) and sodium diethyldithiocarbamate-modified PAC. **T. Kim**, T. Kim, M. Kim, K. Zoh

ENVR 601. Lead and copper ion levels in drinking water: Tap versus bottled. **C. Celani**, P.A. Brletic

ENVR 602. Improving pollution mapping with autonomous and semi-autonoumous vehicles. **J.R. Casar**, G. Quiroz, C.M. Clark, L. Hawkins

ENVR 603. Comparison of effective optical properties of internally mixed aerosols computed using various mixing rules. **K.S. Dooley**, J. DeYoung

ENVR 604. Aerobic granulation for wastewater treatment: Performance evaluation at elevated temperature using real wastewater. **M. Bob**, H. Ab Halim, A. Nor-Anuar, Z. Ujang

ENVR 605. Dechlorination of octachlorodibenzofuran by zero-valent magnesium with and without activated carbon using different solvent systems. **A.T. Mogharbel**, C. Yestrebsky

ENVR 606. Adsorption mechanism of thallium(I) by smectite. **L. Guo**, H. Lin, **S. Wang**

ENVR 607. *In situ* remediation of poly-chlorinated biphenyl contaminated concrete using non-metal and activated metal treatment systems. **A.M. Almutairi**, C.G. Lewis, C. Clausen, C. Yestrebsky

ENVR 608. Selective removal of radioactive cesium from nuclear waste by zeolites: On the origin of cesium selectivity revealed by systematic crystallographic studies. H. Lee, H. Kim, H. Jeong, M. Park, D. Chung, K. Lee, E. Lee, Y. Kim, J. Kim, **W. Lim**

ENVR 609. Mineralogical studies of precipitates and geochemistry of passive treatment system in Gapjeong Coal Mine, Korea. **J. Kim**, J. Seo, C. Lee, Y. Kim, J. Kim, J. Hyeon

ENVR 610. Study on characterization of magnetized zeolitic materials and recovery from aqueous phase by magnetic separation. H. Kwon, T. Shin, W. Lim, J. Kim, **Y. Kim**

ENVR 611. Epoxides as agents for chemical weapon decontamination and solidification. **D.J. McGarvey**, W.R. Creasy

ENVR 612. Development of engineered surrogate soils. **G. Abdalla**, A. Pandey, B.J. Haywood, S.P. Smith, B. Subramanian, D. Spivak, R.L. Cook

ENVR 613. Synthesis and characterization of organically modified montmorillonite for sequestration of perfluoroalkyl acids in contaminated water. **K. Cooley**, L. MacManus-Spencer, M.E. Hagerman

ENVR 614. Synthesis and characterization of organically modified hectorites for sequestration of perfluoroalkyl acids from drinking water. **A. Pagano**, K. Cooley, L. MacManus-Spencer, M.E. Hagerman

ENVR 615. Evolved gas analysis of the preignition stage of invasive plants of East Texas. **A.D. Trevino**, A.S. Frantzen, M. Tiller, B.P. Oswald

ENVR 616. Application of dispersive pipette extraction in analysis of organic contaminants in water. **H. Guan**, X. Li, W. Huang, Q. Cai

ENVR 617. Concentration exposure effects on the integrative capability of polar organic chemical integrative samplers. **R. Taylor**, V. Toteu Djomte, S.M. Chen, K. Chambliss

ENVR 618. Organic matter size and source in urban systems controls Cu biouptake by *Selenastrum capricornutum*. H. Luan, **T.M. Vadas**, K. Turpin-Nagel

ENVR 619. Monitoring of crop protection chemicals in water: Effects of changing environmental conditions on POCIS sampling rates. **V. Toteu Djomte**, R. Taylor, S.M. Chen, K. Chambliss

ENVR 620. Selective catalytic reduction of NO over $Ce_{0.3}TiO_x$ supported metal oxide catalysts. **Z. Duan**, J. Liu, Z. Zhao

ENVR 621. Synthesis $MnCo_2O_4$ spinel-tpye catalyst doped with alkaline earth metal for the catalytic combustion of soot. **K. Zhao**, Z. Zhao, Y. Wei, Y. Li, R. Li

ENVR 622. Novel SCRPF path with the three-dimensionally ordered macroporous $La_{1-x}K_xMnO_3$ perovskite-type mixed metal Oxides atalysts for the simultaneous removal of PM and NO_x from diesel engin. **R. Li**, Z. Zhao

ENVR 623. Removal and recovery of phosphate from wastewater using novel reusable renewable resource-based nanocomposites. **A. Nakarmi**, T. Viswanathan

ENVR 624. Comparative studies of the treatment of rubber processing effluent with *Moringa oleifera* seed powder and *Jatropha carcus* seed powder as coagulants. **O. Ize-Iyamu**, E. Egbon, D. Ehiwe, O. Ize-Iyamu

ENVR 625. Application of factorial analysis to optimize preparation of activated carbons from renewable and low-cost precursors including olive pits, date pits, acorn shells, corn husks and coconut shells. **A. Algahamdi**, Z. Al-Khayat, A. Almalki, A. Alrashdi, T. Assiri, E. Alkhatib, P.A. Snetsinger

Section A
Ernest N. Morial Convention Center
Hall D

Green Chemistry & the Environment

A. Balu, R. Luque, S.O. Obare, *Organizers*

6:00–8:00

ENVR 626. 2D material-based membranes for ionic liquid recycling. **J. Yin**, S. Tan, I. Hammontree, D. Li

ENVR 627. Beyond palm oil: Anticipatory environmental and techno-economic modelling for a bio-refinery process producing future food, fuels and high-value chemicals using green chemistry techniques. **S. Parsons**, M. McManus, C. Chuck

ENVR 628. Absorption of lactic acid from fermentation broth using a cost-effective adsorbent. **K. Chutivasanaskun**, T. Chaisuwan, S. Wongkasemjit

ENVR 629. Ecological friendly fabrication of polymer composites employing solution blending assisted with protic ionic liquid. **R.L. Perez**, J.S. Van Buskirk, P.K. Chhotaray, I.M. Warner

ENVR 630. Impacts of energy on environment. **T. Komolafe**

ENVR 631. Novel discharge-based technology for converting tar compounds into fuel gas. **J. Sun**

ENVR 632. Withdrawn.

ENVR 633. Using enzymatic combinations to treat asphaltene aggregation. **J. Abolafia**, **J. Cowan**, **A. Harrison**, **J. Hensley**, **T. Kim**, **W. Ko**, **M. Le**, **H. Manivannan**, **L. Rivera**, **P. Sarker**, **R. Tyagi**

Section A
Ernest N. Morial Convention Center
Hall D

Innovative Chemical & Material Approaches for Sustainable Water Purification

J. Choe, J. Liu, D. Shuai, Y. Wang, *Organizers*

6:00–8:00

ENVR 634. Mechanistic study on the decomposition of perfluorooctanesulfonic acid by advanced oxidation combined with reductive defluorination. **N. Souza**, A. Parenky, H. Choi

ENVR 635. Functionalized chitosan-$Ti_3C_2T_x$ (MXene) nanofiber composite for water filtration. **E. Mayerberger**, A. Toth, M. Barsoum, C.L. Schauer

ENVR 636. Effects of citrate and tartrate on 2,4-dichlorophenol and 2,4,6-trichlorophenol removal in pyrite-packed columns under continuous flow conditions using heterogeneous Fenton reaction. O. Oral, **C. Kantar**, N.A. Oz

ENVR 637. Development of functional plastics containing long-chain aliphatic podands for the remediation of water. **J. Pothoof**, M. Bhagwagar, C. Baker, M.A. Benvenuto

ENVR 638. Air cathode iron-electrocoagulation (ACE) for removing emerging contaminants of concern in wastewater. **S. Bandaru**, A. Gadgil

ENVR 639. Utilization of polyisobutylene bound magnetic nanoparticles for the extraction of crude from aqueous environment conditions. **P.K. Manyam**

ENVR 640. Faceted TiO_2/Fe_2O_3 nanoparticles with carbon-based supports for water treatment applications. **A. Yurum**, Z. Gohari, Y. Yurum

ENVR 641. Adsorption technique for organic pollutants using different carbon materials. **A. Mahmoud**, A. Stolle, M. Stelter, P. Braeutigam

ENVR 642. Hybrid porous materials for the removal of dye-contaminated wastewater. **M. Chin**, F. Tian

ENVR 643. Adsorption of lead onto activated carbon derived from *Garcinia cambogia*. **A. Liyanage**, M. Edussuriya, T. Mlsna

ENVR 644. Withdrawn.

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ENVR 645. Innovative chemical & material approaches for sustainable water purification. **S. Goodman**, K. Song, A. Dichiara

Section A
Ernest N. Morial Convention Center Hall D

Novel Concepts in the Role of Chemistry in the Food, Energy & Water Nexus

S. Ahuja, S. Chae, I. Chowdhury, D.D. Dionysiou, *Organizers*

6:00–8:00

ENVR 646. Discovery of design principles for phosphate recognition at water interfaces. **W. Zhao**, J.F. Neal, H.C. Allen, A.H. Flood

ENVR 647. Extraction and quantification of environmental inositol phosphates using solid phase extraction and inductively coupled plasma mass spectroscopy. **A. Altomare**, M.J. Beazley

ENVR 648. Diurnal variability in organic matter constituents in an anaerobic baffled reactor treating domestic wastewater for agricultural water reuse applications. Z. Orandle, B. Pietruschka, M. Palomo, C. Buckley, S. Mncumbe, C. Pascua, L. Steinberg, **N. Mladenov**

Section A
Ernest N. Morial Convention Center Hall D

Novel Membrane-Based Technology for Water Purification & Desalination

D. Jassby, B. Mi, *Organizers*

6:00–8:00

ENVR 649. Removal of natural organic matter with nano-filtration after electrodialysis pretreatment. **S. Kum**, D.F. Lawler, L.E. Katz

ENVR 650. Mitigation of toxic industrial chemicals and materials in water for emergency individual hydration. **E. Brack** , W. Zukas, T. Tiano, M. Mcpartlin

ENVR 651. Effect of the surface zeta potential on the fouling reduction of nanocellulose coated ultrafiltration membranes. **M. Yang**, B.S. Hsiao, P. Hadi

ENVR 652. Analysis of organic compound permeability in relation to ultrafiltration membrane fouling. **A.A. Sanchez**, N. Mladenov

Section A
Ernest N. Morial Convention Center Hall D

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern

L.M. Blaney, A.J. Hernandez, A. Heyden, Y. Men, *Organizers*

6:00–8:00

ENVR 653. Effect of iron activator types on the persulfate oxidation of pharmaceuticals (diclofenac, salicylic acid and ibuprofen). **J. Choi**, W. Sik Shin

ENVR 654. Role of morphology and corresponding properties in nanotoxicity of nanoscale battery material $Li_xNi_yMn_zCo_{1-y-z}O_2$. **N.V. Hudson-Smith**, M. Hang, P. Clement, R.J. Hamers, C.L. Haynes

ENVR 655. Exploring the role of lipopolysaccharides in bacterial interactions with nanoparticles. J.T. Buchman, A. Rahnamoun, **K.M. Landy**, X. Zhang, A. Vartanian, L.M. Jacob, C.J. Murphy, R. Hernandez, C.L. Haynes

Section A
Ernest N. Morial Convention Center Hall D

Physics & Chemistry of Water Treatment: Symposium in honor of Professor Desmond F. Lawler

J. Darby, L.E. Katz, J.A. Nason, N.B. Saleh, *Organizers*

6:00–8:00

ENVR 656. Quantifying copper speciation in pulp and paper wastewater effluent and implications for the biotic ligand model. **J. Mitzel**

ENVR 657. Examining the role of TiO_2 surface transformations on nanoparticle properties and treatment efficacy. **A. Deline**, J.A. Nason

ENVR 658. Fundamental studies of ultrasound induced degradation of a popular antihistamine, cetirizine. **D. Cui**, A. Tarifa, A. De Caprio, K.E. O'Shea

ENVR 659. Predicting performance and nutrient management feasibility of struvite recovery systems. **A. Furneaux**, R.D. Cusick

ENVR 660. Impact of water quality characteristics on the mitigation of estrogenic contaminants from drinking water via electrocoagulation and electrooxidation. **K.N. O'Malley**, E. Maher, P. McNamara

ENVR 661. Aqueous chloride concentrations and ionic strength control silver nanoparticle toxicity in *Pseudomonas aeruginosa* thereby increasing stress response and antibiotic resistance. **B.A. Chambers**, S.K. Smith, N.B. Saleh, M.J. Kirisits

ENVR 662. Forward osmosis on seawater and wastewater effluent from a steel industry. J. Jung, **J. Kweon**, J. Ryu

ENVR 663. Modeling the performance of a pulp mill wastewater treatment plant located in Uruguay, South America. S. Bentancur, C. Lopez-Vazquez, **H. Garcia**, M. Duarte, D. Brdjanovic

ENVR 664. Biosolids-derived biochar for adsorption of organic micropollutants: The impact of temperature and pore size. **Y. Tong**, B. Mayer, S.L. Singer, P.J. McNamara

ENVR 665. Physicochemical relationships between metal-based (Fe^{3+}, Al^{3+}) precipitates and inorganic/organic contaminants. **S. Yeo**, T. Stewart, S. Yoon, D.F. Lawler, L.E. Katz

ENVR 666. Influence of coagulant characteristics on the removal of DOM and low levels of Hg from surface water in alum and ferric-coagulation systems. **F. Diaz**, L.E. Katz, D.F. Lawler

ENVR 667. Effect of sludge retention time on the filtration performance of anaerobic membrane bioreactors treating synthetic dairy wastewater with high lipid content. **A. Szabo**, S. Pacheco-Ruiz, D. Miguez, C. Hooijmans, H. Garcia, D. Brdjanovic, J. van Lier

ENVR 668. Evaluation of the Speece cone oxygen transfer performance in clean water and mixed liquor in a pilot-scale membrane bioreactor. M. Barreto, I. Ochoa, **H. Garcia**, C. Hooijmans, D. Brdjanovic

ENVR 669. Predicting electro conductivity based on ionic composition for multi component aqueous solutions. **S. Jafarzade Ghadimi**, W. Walker

ENVR 670. Achieving high water recovery in real brackish water treatment by membrane capacitive deionization (MCDI) desalination systems. **O. Owoseni**

ENVR 671. Relative importance of sweep coagulation and inactivation for virus control at different pH values during iron electrocoagulation. **K. Kim**, S. Chellam

ENVR 672. Constant flux microfiltration of secondary wastewater effluent: Fouling mechanisms with and without backwashing. **K. Gupta**, S. Chellam

ENVR 673. Performance deterioration and chemical cleaning of 7-year old reverse osmosis membranes from a full-scale water reuse facility. **B. Abada**, S. Chellam

ENVR 674. Transformation and aggregation of indium tin oxide (ITO) nanoparticles: Influence of surface chemistry on environmental fate of globally important engineered nanomaterial. **J. Grundy**, A. Suresh, N.B. Saleh, L.E. Katz, C.A. Saez Cabezas, M.J. Kirisits, D.J. Milliron

ENVR 675. Ultrasonic degradation of the Zika pesticide naled in aqueous solution: Kinetics and mechanistic investigation. **A. Abdullah**, K.E. O'Shea

Section A
Ernest N. Morial Convention Center Hall D

Redox & Interfacial Dynamics Among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients

J.M. Cerrato, Y. Hu, Z. Wang, T. Zeng, *Organizers*

6:00–8:00

ENVR 676. Dynamic interaction between As, Fe, and S controlling arsenic mobility. **T. Jiarong**, C. Liu, L. Peng

ENVR 677. Interaction between reduced colloidal humic substances with chromium and its effect on chromim transformation and transport. **B. Li**, C. Liu, P. Liao

ENVR 678. Dechlorination reactivity of biologically derived iron sulfide and sulfidated zero-valent iron particles. **A.W. Murray**, S. Islam, W. Yan, K. Millerick

ENVR 679. Preparation of magnetic chitosan honeycomb beads composed of chitosan and sodium citrate: an effective and recyclable adsorbent for the removal of heavy metal ions from aqueous solutions. **S. Pu**, H. Ma, **W. Chu**

ENVR 680. NOx and SOx formation, reaction, and dispersion in complex urban areas: Modeling and comparison to field data. **S. Wuerz**

Section A
Ernest N. Morial Convention Center Hall D

Shaping Activity through Structural Modification: From Small Molecules to Nanoparticles: A Symposium in honor of Professor Bing Yan

D.D. Dionysiou, V.K. Sharma, H. Zhou, *Organizers*

6:00–8:00

ENVR 681. Breakdown of TCDD using a visible light-powered hybrid photocatalyst (FePWC3N4): Detection with residual toxicity to zebrafish embryos. A. Wang, Z. Wang, W. Dong, J. Dong, J. Liu, D.E. Hinton, M. Chernick, **W. Dong**

ENVR 682. GD2-targeting nanoconstruct as CT imaging and NK cell-mediated cancer cell killing agent. **P. Jiao**

ENVR 683. Amidoximes as histone deacetylase inhibitors. **Q. Geng**

ENVR 684. Two of the seven nanoparticle properties induce oxidative stress through distinct pathways. H. Sun, **H. Zhou**, B. Yan

ENVR 685. Airborne particulate matter causes the activation of plasma kallikrein-kinin system. **Q.S. Liu**, X. Jin, F. Hao, Q. Zhou, G. Jiang

ENVR 686. Formation of environmentally persistent free radicals (EPFRs) on polycyclic aromatic hydrocarbons (PAHs) contaminated ion metals modified-smectite clays. **H. Jia**

ENVR 687. Protein corona formation ameliorate amorphous silica nanoparticle-induced cardiovascular inflammation. **Y. Song**

Section A
Ernest N. Morial Convention Center Hall D

Water Use Optimization: Water Quality, Reuse & Treatment

S. Bushart, Y. Jun, K. Pagilla, N. Rao, Y. Yang, *Organizers*

6:00–8:00

ENVR 688. Withdrawn.

ENVR 689. Trace metal quantification in unregulated water sources on the Navajo Reservation. **J. Torkelson**, J. Credo, J.C. Ingram

ENVR 690. Removal of bisphenol-S (BPS) by O_3 and H_2O_2 advanced oxidation processes in water. **C. Weeks**, P.A. Ruiz-Haas

ENVR 691. Polymeric membrane reactor for ozone treatment of endocrine disrupting compounds in water. Y. Li, **J. Song**, K. Yeung

ENVR 692. Microwave–induced catalytic oxidation of two–component (phenol, p–nitrophenol) phenolic

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wastewater. R. Liu, W. Wang, C. Shi, **C. Ma**

Biomineralization & Bio-Compatible Minerals
Sponsored by GEOC, Cosponsored by BIOL and ENVR

Contaminated Site Remediation through Microbial, Geological & Chemical Processes
Sponsored by GEOC, Cosponsored by ENVR

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Forensic Geochemistry
Sponsored by GEOC, Cosponsored by ENVR

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Sponsored by GEOC, Cosponsored by ENVR

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Sponsored by GEOC, Cosponsored by BIOL and ENVR

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Sponsored by GEOC, Cosponsored by ENVR

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments
Sponsored by GEOC, Cosponsored by ENVR and INOR

Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes
Sponsored by GEOC, Cosponsored by AGRO and ENVR

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Sponsored by GEOC, Cosponsored by ENVR and INOR

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 346

Green Chemistry & the Environment
Cosponsored by CEI
Financially supported by AEESP
A. Balu, S.O. Obare, *Organizers*
R. Luque, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 693. Recovery of rare earth elements (REEs) from coal fly ash: Coupling hydrothermal extraction and ligand-associated hydrophobic glass media sorption. **T.M. Dittrich**, S.K. Mohanty

9:05 ENVR 694. Voided polymer imaging technology for thermal printing. **B. Einsla**

9:35 ENVR 695. Alternative solvents in organic synthesis: Supporting the incorporation of sustainability into the chemical industry. **K.L. Wilson**, A.J. Watson

10:05 ENVR 696. Chemical innovation: A GAO report on sustainability. **K. Howard**

10:25 Intermission .

10:35 ENVR 697. Dual optimization of microporosity in carbon spheres for superior CO_2 adsorption at ambient conditions. **A.C. Dassanayake**, M. Jaroniec

10:55 ENVR 698. Adsorption of bisphenol-A in aqueous solution using silica nanoparticles obtained from sugarcane waste ash. **S. Rovani**, J.J. Santos, P. Corio, D.A. Fungaro

11:15 ENVR 699. Reduction of Pb and Cr metal contents in laboratory wastewater using electrocoagulation and chelation of citric acid from *Averrhoa bilimbi*. Linn. **C. Safitri**, Y. Yusbarina

11:35 ENVR 700. Microwave-induced organic synthesis and mass spectral characterization of curcumin and 2-aminoguanidine adduct: A potentially useful inhibitor for advanced glycation end products in diabetes and other chronic diseases associate with oxidative stress. **B. Dayal**, M.A. Lea

11:55 ENVR 701. Environmentally persistent free radicals in total particulate matter of tobacco smoke and e-cigarettes. **F. Hasan**, L. Khachatryan, S.M. Lomnicki

12:15 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
Room 347

Current State of Environmental Contamination Research: Theory & Experiment
Cosponsored by CEI
S. Ahuja, M.K. Shukla, *Organizers*
G. Jenness, H. McAlexander, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 702. Environmental organic chemistry: Photooxidation and fate transport. **W. Nelson**

8:30 ENVR 703. Photocatalytic nylon: Chitosan membrane blends. **J.P. Buchanan**, C.A. Weiss, J.A. Jefcoat, H.R. Peel, R.K. Buchanan, A.D. Netchaev, J.D. Klein, S.G. Patel, R.D. Brown, J.M. Montijo

8:55 ENVR 704. Biodegradation of environmental microplastics generated from laundering of fabrics. **J. Pawlak**, R.A. Venditti, J. Daystar, M. Ankeny, J. Cheng

9:20 Intermission.

9:35 ENVR 705. Degradation kinetics of tetracycline antibiotics in agricultural manure during anaerobic digestion. **J. Kasumba**, B. Couch, J.H. Loughrin, E.D. Conte

10:00 ENVR 706. Predicting thermophysical properties of environmental contaminants via first principles and classical molecular simulation approaches. **N. Rai**, H. Goel, S. Venkatesan

10:25 ENVR 707. Nature of contaminants in arid soil: A computational study on the adsorption of munition compounds and arsenic species on the (0001) surface of β-Fe_2O_3 and β-Al_2O_3. **G.R. Jenness**, J. Seiter, M.K. Shukla

10:50 Intermission.

11:05 ENVR 708. Mechanistic insights into the aerobic oxidation of alcohols on Pd(111). **J.R. Schmidt**

11:30 ENVR 709. Quantum chemical calculation on photodegradation of some insensitive munitions compounds. **M.K. Shukla**

Section C
Ernest N. Morial Convention Center
Room 348

Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery
Cosponsored by CEI
Y. Men, C.M. Sales, *Organizers*
X. Mao, S. Yi, W. Zhuang, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 710. Locally enriched cultures can cometabolize 1,4-dioxane at drinking water relevant concentrations. **A. McElroy**, D. Knappe, M. Hyman

8:25 ENVR 711. Cometabolic degradation of antibiotic using microalgae. **J. Xiong**, M. Kurade, G. Ha, J. Kim, B. Jeon

8:45 ENVR 712. Ammonia-monooxygenase-mediated cometabolic biotransformation and abiotic transformation of micropollutants. **Y. Yu**, P. Han, L. Zhou, M. Wagner, Y. Men

9:05 ENVR 713. Biotransformation of 6:2 fluorotelomer thioether amido sulfonate under different redox conditions. **S. Yi**, K. Harding-Marjanovic, E. Houtz, J.A. Field, W. Zhuang, D.L. Sedlak, L. Alvarez-Cohen

9:25 ENVR 714. Microbial community variation in organohalide antibiotics containing waterbodies. **J. He**

9:55 Intermission.

10:10 ENVR 715. Biocatalytic degradation of 1,2,3-trichloropropane for achieving extremely low regulatory limits. **A. Razavi**, F. Shirazi

10:30 ENVR 716. Surface display enzyme biocatalysts for treating emerging contaminants. **N. Wei**, Y. Chen, B. Zhu

10:50 ENVR 717. Identification and enzymatic characterization of a novel NADH dependent azoreductase, encoded by *AzoK* in *Klebsiella pneumoniae*. **S. Dixit**, S. Garg

11:10 ENVR 718. Polycyclic aromatic hydrocarbon degradation by *Cycloclasticus*, as measured by a novel immunoassay, correlates with increased cell proliferation. S. Zhang, M. Omarova, L. Swientoniewski, A. Panchal, T. Yu, V.T. John, Y. Lvov, D. Zhang, **D.A. Blake**

11:30 ENVR 719. From bioavailability science to soil remediation: Sustainable stimulation of biological networks for enhanced pollutant carbon turnover. **J. Ortega-Calvo**, R. Posada-Baquero, J. Vila, J. Garcia, M. Cantos

Section D
Ernest N. Morial Convention Center
Room 349

Water Use Optimization: Water Quality, Reuse & Treatment

Water treatment: Processes

S. Bushart, Y. Jun, K. Pagilla, N. Rao, Y. Yang, *Organizers, Presiding*

8:00 ENVR 720. Impact of CeO_2 nanoparticles and sodium chloride (NaCl) on soil water potential and distribution. B.L. Hallmark, X. Ma, A. Assi, P. Schwab, **R. Mohtar**

8:30 ENVR 721. Source water quality impacts on drinking water treatment plant performance and disinfection byproduct formation during a storm event. **C.W. Neil**, Y. Zhao, A. Zhao, J. Neal, J. Yang

8:50 ENVR 722. Investigation of radical chlorine species in advanced oxidation processes. **J. Castillo**, S. Mezyk

9:10 ENVR 723. Treatability of dissolved organic nitrogen in an advanced tertiary wastewater treatment plant. **K. Ahmadi**, A. Mayorga, Y. Yang, E. Marchand

9:30 ENVR 724. Formation of bromated halonitromethanes from organic amines during ozonation. **J. Fu**, H. Yang, X. Wang, J. Tan, W. Yuan, Z. Yuan, L. Feng, Y. Xie

9:50 Intermission.

10:00 ENVR 725. Withdrawn

10:20 ENVR 726. Evolutionary trajectories of urban water demand and the journey towards the water sensitive city. **M. Rippy**

10:40 ENVR 727. Impact of operating conditions in membrane-based separation processes on the characteristics of inorganic scales on membrane surface. **O.R. Lokare**, S. Wadekar, R.D. Vidic

11:00 ENVR 728. pH-dependence of chloramine photolytic quantum yields under advanced oxidation process conditions. **L. Twight**, K.P. Ishida, S.P. Mezyk

11:20 ENVR 729. Radical-based degradation of contaminant alkyl nitrates in advanced oxidation process treated wastewaters. **S. Arciva**, B. Daws, S.P. Mezyk

11:40 ENVR 730. Investigation of the reaction of the hypochlorite radical with nitrosamines in aqueous solution. **A. Lechner**, S.P. Mezyk

Section E
Ernest N. Morial Convention Center
Room 350

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

T. Anumol, R. Marfil-Vega, T.M. Young, C. Zwiener, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ENVR 731. Structure identification by mass spectrometry non-targeted analysis using the US EPA's CompTox Chemistry Dashboard. **A.J. Williams**,

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A. McEachran, C. Grulke, S. Newton, K. Isaacs, K. Philips, N. Baker, J. Sobus

8:30 ENVR 732. Quality control/quality assurance for qualitative analysis of environmental samples by LC/HRAM MS. **J. Zweigenbaum**

8:55 ENVR 733. Exploring the exposome with non-targeted analysis of house dust. **E.M. Ulrich**, D. Mills, J. Sobus, J. McCord, K. Hibbert, N. Tulve

9:20 ENVR 734. Comprehensive targeted and non-targeted analysis of indoor dust using LC-HRMS with ion mobility. **D. Stevens**, L. Mullin, K. Jobst, E. Reiner, A. Ladak, R. Plumb

9:45 Intermission.

10:10 ENVR 735. Developing and improving accurate mass tools for the analysis of unknowns in surface and groundwater samples. **E.M. Thurman**, I. Ferrer, J. Zweigenbaum

10:35 ENVR 736. Kendrick mass defect as an additional tool to process high resolution mass spectrometry data and identify transformation products. **C. Zwiener**, S. Merel

11:00 ENVR 737. Identifying universally present consumer product constituents in California sewage sludge by high resolution LC-ESI-qTOF-MS. **G. Pecora**

11:25 ENVR 738. Hydrogen deuterium exchange of environmental samples to improve non-target elucidation. **E. Schymanski**, C. Ruttkies, J. Hollender, S. Neumann, M. Krauss

11:50 Discussion.

Section F
Ernest N. Morial Convention Center
Room 351

Nutrient Management & Water/ Wastewater Treatment through Biomass Production in Aquatic & Terrestrial Ecosystems

W. Grieco, A. McQuilling, *Organizers, Presiding*

9:00 Introductory Remarks.

9:05 ENVR 739. Efficacy of submerged attached growth reactors for small community wastewater ammonia removal. **R.R. Mattson**, M. Wildman, C.L. Just

9:25 ENVR 740. Integrating anammox with autotrophic denitrification process by electrochemistry technology. **S. Qiao**, X. Yin, J. Zhou

9:45 ENVR 741. Electrocatalytic oxidation degradation of ammonia nitrogen wastewater. **Z. Yang**, G. Yan, S. Guo

10:05 ENVR 742. Comparative assessment of suspended and benthic microalgae cultivation stragetgies for water treatment and production of biobased commodities. **R.W. Davis**, A. Siccardi, J. Quinn, R.C. Pate

10:25 Intermission.

10:40 ENVR 743. Modeling nitrogen use efficiency in multi-trophic aquaculture production. **A. McQuilling**, D. Blersch, D. Wells

11:00 ENVR 744. Conversion of concentrated thin stillage from corn-ethanol production to beneficial biomass products. **C. Lin**, P. K C, K. Gurung, S. Shatu, T. Mccawley, R.G. Jones, B. Corace, E. Corace, C. Lin

11:20 ENVR 745. Optimized combination of fillers in constructed wetlands for eutrophication control. **Z. Duan**, Q. Liu, J. Liu, G. Wang, Y. Zhou, H. Liu, N. Li

11:40 ENVR 746. Resource recovery from wastewater as single-cell protein. **H.R. Molitor**, J.L. Schnoor

Section G
Ernest N. Morial Convention Center
Room 342

Advances in Understanding of Sorptive & Reactive Properties of Pyrogenic Carbonaceous Matter (PCM) in the Environment

W. Mitch, J.J. Pignatello, *Organizers*
W. Xu, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENVR 747. Pyrogenic carbonaceous matter interactions with inorganic and organic carbon and nitrogen. **J. Lehmann**, R. Hestrin, L. Krounbi, S. DeCiucies, T. Whitman

9:10 ENVR 748. Biochars change the sorption and degradation of thiacloprid (THI) in soil: Insights into chemical and biological mechanisms. **H. Sun**, P. Zhang

9:30 ENVR 749. Carbon dioxide-mediated ammonia loading onto pyrogenic waste biomass. **L. Krounbi**

9:50 Intermission.

10:05 ENVR 750. Pyrogenic organic matter alters the efficiency of soil microbial communication. **C.A. Masiello**, X. Gao, H. Cheng, V.I. Del, J.J. Silberg

10:40 ENVR 751. Influence of black carbon on anaerobic microbial dechlorination rates of PCBs. **T. Needham**, U. Ghosh, K.R. Sowers

11:00 ENVR 752. Biochar-facilitated microbial reduction of hematite. S. Xu, D. Adhikari, R. Huang, Y. Tang, E.E. Roden, **Y. Yang**

11:20 Panel Discussion.
11:40 Concluding Remarks.

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Sponsored by GEOC, Cosponsored by ENVR

Elucidation of Mechanisms & Kinetics on Surfaces
Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Lignin: From Fundamentals to New Materials & Applications

Polymers & Resins from Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Iron Oxyhydr-Oxides: Redox Processes

Sponsored by GEOC, Cosponsored by ENVR and INOR

Unconventional Catalysis Targeting Stable Molecules
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

THURSDAY AFTERNOON

Section B
Ernest N. Morial Convention Center
Room 347

Current State of Environmental Contamination Research: Theory & Experiment
Cosponsored by CEI
S. Ahuja, G. Jenness, *Organizers*
H. McAlexander, M.K. Shukla, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENVR 753. City-specific *in vitro* exposure-toxicity relationships of $PM_{2.5}$ in China. **L. Jin**, J. Xie, C.K. Wong, R. Zimmermann, X. Li

1:30 ENVR 754. Assessing the impacts of changes in sources on air pollution in Rochester, NY from 2008 to 2013. **F. Emami**, P. Hopke

1:55 ENVR 755. Environmental remediation of chlorinated hydrocarbons using biopolymer stabilized iron loaded halloysite nanotubes. **Y. Su**

2:20 Intermission.

2:35 ENVR 756. Synthesis and evaluation of novel low viscosity amine-based acid gas capture solvents. **J. Page**, D. Malhotra, P.K. Koech, M. Nguyen, R. Zheng, V. Glezakou, R. Rousseau, D.J. Heldebrant

3:00 ENVR 757. Intra-day pollution characteristics and load investigation of antibiotics in major wastewater treatment plants of Beijing based on a more reliable sampling approach. **Y. Zhang**, B. Wang, G. Yu

3:25 ENVR 758. Biogeochemical model for gas ebullition in the presence of NAPLs in sediments. **M. Khazraee Zamanpour**, **K. Rockne**

3:50 Intermission.

4:05 ENVR 759. Toward quantitative $H_2PO_4^-$ sensing: Simultaneous determination of all species concentrations in multi-equilibria of aqueous solutions containing dihydrogen phosphate. **J. Schell**, E. Zars, C. Chicone, R. Glaser

4:30 ENVR 760. Source identification of fluorescent dissolved organic matters in MX river by PARAFAC and HPSEC. **B. Liu**, J. Wu, C. Cheng, J. Tang, Y. Chai, M. Khan

4:55 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 348

Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery
Cosponsored by CEI
Y. Men, S. Yi, *Organizers*
X. Mao, C.M. Sales, W. Zhuang, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENVR 761. Green oxidation via bioelectrochemically derived hydrogen peroxide. **J. Griffin**, E. Taw, A.A. Gosavi, N. Thornburg, K.A. Gray, J.M. Notestein, G. Wells

1:25 ENVR 762. Combining bioremediation and in situ chemical oxidation for treatment of aqueous film forming foams (AFFFs) in groundwater. **E.K. Cook**, Y. Sun, **C.I. Olivares**, S. Yi, D.L. Sedlak, L. Alvarez-Cohen

1:45 ENVR 763. Bioelectrochemical treatment of mixed 1,4-dioxane and chlorinated solvent contaminations. **N. Pica**, N. Johnson, Y. Miao, S. Mahendra, J. Blotevogel

2:05 ENVR 764. Lab-scale continuous ozonation combined with biofiltration to understand the fate of trace contaminants during slow sand filtration and soil aquifer treatment. **J. Wenk**, G. Zoumpouli, B. Kasprzyk-Hordern, O. Happel

2:25 ENVR 765. Deciphering microbial phenotypes via isotopically nonstationary metabolic flux analysis. **Y. Tang**

2:55 Intermission.

3:05 ENVR 766. Mass balance for N transformations in a nitrogen removing biofilters for onsite residential wastewater treatment. **S. Waugh**, X. Mao, C.J. Gobler, H. Walker

3:35 ENVR 767. Biofilm biology-informed biofilm engineering for environmental applications: From understanding biofilm lifestyle to building a better biofilm. Y. Wu, M. Mukherjee, **B. Cao**

3:55 ENVR 768. Withdrawn.

4:15 ENVR 769. Integrated system for thin stillage remediation coupled with microalgae cultivation for carbohydrate production. F. Sayedin, **A. Kermanshahi Pour**, Q. He

4:35 ENVR 770. Electrochemical filters for the selective recovery of rare earth and specialty metals. **D.L. Plata**, M.P. O'Connor

Section D
Ernest N. Morial Convention Center
Room 349

Water Use Optimization: Water Quality, Reuse & Treatment

Water treatment: Method development

S. Bushart, Y. Jun, K. Pagilla, N. Rao, Y. Yang, *Organizers, Presiding*

1:00 ENVR 771. Multi-scale systems analysis for engineering optimization in water supply infrastructure systems. **Y. Yang**, C. Neil, N. Chang, Y. Jun, **B. Bierwagen**, T. Speth

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1:30 ENVR 772. High frequency and near real-time monitoring of N-nitrosodimethylamine using a novel extraction-free chemiluminescence-based method. **S. Roback**, M.H. Plumlee, K.P. Ishida, T. Fujioka, H. Kodamatani

1:50 ENVR 773. Evaluation of the formation of chlorinated by-products during surface water treatment by an electro-peroxone process. **W. Yao**, J. Fu, G. Yu, Y. Wang

2:10 ENVR 774. Establishing cost and performance goals for electrochemical deionization: A techno-economic analysis of faradaic and capacitive materials in CDI systems. **S. Hand**, X. Shang, K. Smith, R.D. Cusick

2:30 ENVR 775. Slow-release persulfate candle assisted electrochemical oxidation of PAHs in groundwater. **A. Sarmanik**, W. Sik Shin

2:50 Intermission.

3:05 ENVR 776. Photocatalytic degradation of disinfection byproducts using natural sunlight and TiO_2. **I. Abusallout**, G. Hua

3:25 ENVR 777. Peanut shell based activated carbon and its use for heavy metal removal. **D. Pitre**, M. Edussuriya, T. MIsna

3:45 ENVR 778. Competitive association of scale-forming cations with different water-soluble anionic polyelectrolytes (PSS and PAA) during membrane separation. **M. Chen**, K. Shafer-Peltier, S. Randtke, E.F. Peltier

4:05 ENVR 779. Adsorption kinetics of 4-n-nonylphenol on hematite and goethite. **K. Watson**

Section E
Ernest N. Morial Convention Center
Room 350

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

T. Anumol, R. Marfil-Vega, T.M. Young, C. Zwiener, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 ENVR 780. Fall Creek monitoring station: An automated workflow to identify emerging contaminants using highly resolved temporal sampling. **C. Carpenter**, D.E. Helbling

1:30 ENVR 781. Identification of micropollutants in surface water by using suspect screening strategies based on regulatory databases. **P. Gago-Ferrero**, A. Krettek, L. Ahrens, K. Wiberg

1:55 ENVR 782. Tracking large numbers of CECs via non-target screening. **K.S. Jewell**, C. Dietrich, U. Kunkel, M. Schluesener, U.R. Thorenz, F. Thron, T. Ternes

2:20 ENVR 783. Emerging micropollutants in environment: Analysis of water samples by high resolution mass spectrometry. **M. Chachignon**, E. Cocardon, M. Denieul, V. Ingrand, G. Leroy, G. Meheut, C. Tondelier

2:45 Intermission.

3:10 ENVR 784. Detecting polar micropollutants in a river-riverbank filtrate using non-target screening. **V. Albergamo**, J. Schollee, E. Schymanski, R. Helmus, J. Hollender, P. de Voogt

3:35 ENVR 785. Suspect screening of halogenated micropollutants in surface waters affected by wastewater discharges using passive samplers. **F. Menger**, K. Wiberg, L. Ahrens, P. Gago-Ferrero

4:00 ENVR 786. Targeted and untargeted analysis of per- and polyfluoroalkyl substances in Australian wastewater treatment plants. T. Coggan, T. Anumol, J. Shimeta, N. Crosbie, C. Milner, **B. Clarke**

4:25 ENVR 787. Newly identified hydrocarbon surfactants in AFFFs and AFFF-impacted groundwater. **R.A. Garcia**, A.C. Chiaia Hernandez, P. Lara-Martín, M. Loos, J. Hollender, J.A. Field

4:50 Concluding Remarks.

Elucidation of Mechanisms & Kinetics on Surfaces
Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Sponsored by GEOC, Cosponsored by ENVR

Lignin: From Fundamentals to New Materials & Applications

Biochemical Modification of Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Uranium Incorporation: Sulfate Mineral Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Sponsored by GEOC, Cosponsored by ENVR and INOR

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

FLUO

Division of Fluorine Chemistry

N. Vasdev, *Program Chair*

SUNDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Erhard Kemnitz

T. Braun, D.A. Dixon, *Organizers*
F. Kraus, T. Skapin, *Presiding*

8:00 Introductory Remarks.

8:10 FLUO 1. Oxidations of aromatic species, usually in HF. **K. Seppelt**, M. Malischewski, M. Khanfar

8:40 FLUO 2. Coordination chemistry of xenon(VI) trioxide. **G.J. Schrobilgen**, J.T. Goettel, K.M. Marczenko, V. Haensch, H. Mercier

9:10 FLUO 3. Silicon fluorides and their congeners. **H.W. Roesky**

9:40 Intermission.

10:00 FLUO 4. Computational characterisation of catalysts in reactive environments: Phase stability, surface compostion, structure and reaction sites. **N. Harrison**

10:30 FLUO 5. Employing silylium-ion like surface species as a potent hydrodehalogenation catalyst. **M. Ahrens**, M. Feist, A. Siwek, T. Braun, E. Kemnitz

11:00 FLUO 6. Novel synthesis approaches towards *nano* copper(II) fluoride – a high potential material for lithium ion batteries. **T. Krahl**, F. Marroquin Winkelmann, A. Martin, E. Kemnitz

SUNDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Erhard Kemnitz

T. Braun, D.A. Dixon, *Organizers*
M. Finze, G.J. Schrobilgen, *Presiding*

1:00 FLUO 7. Fluoroammonium cations. **K.O. Christe**, A. Vij, W. Wilson, R.M. Haiges, D.A. Dixon

1:30 FLUO 8. Solid-state structure of protonated ketones and aldehydes. **M. Gerken**, D. Stuart, S.D. Wetmore

2:00 FLUO 9. New superacids based on pentafluoroorthotellurate derivatives of aluminium. **S. Riedel**

2:30 Intermission.

2:50 FLUO 10. Recent studies on direct fluorinations and fluoroalylations. **S.S. Prakash**

3:20 FLUO 11. NHC-nickel-catalyzed derivatization of polyfluoroarenes via nickel-mediated C-F bond cleavage. **U. Radius**

3:50 FLUO 12. Synthesis and reactions of aryldifluoromethyl copper reagents. M. Kathan, B. Duda, A. Haupt, **D. Lentz**

4:20 FLUO 13. Methylation of nitriles: Isolation and characterization of N-methyl nitrilium ions. **T. Saal**, A. Nitzer, K.O. Christe, R.M. Haiges

MONDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Erhard Kemnitz

T. Braun, D.A. Dixon, *Organizers*
M. Gerken, S.S. Prakash, *Presiding*

8:00 FLUO 14. Fluorine-containing matrix-metalloproteinase inhibitors: The role of Fluorine substituents and Zinc binding groups on activity. **G. Haufe**

8:30 FLUO 15. Preparation and reactivity of selected cross-conjugated fluoro-isoindenones and fluoro-dendralenes. **M. Etzkorn**

9:00 FLUO 16. Fluorine in peptide and protein engineering. **B. Koksch**

9:30 FLUO 17. Interaction of genetically engineered polypeptides with rare earth-containing metal fluoride nanoparticles. J.P. Seeley, T. Krahl, E. Kemnitz, **J.T. Welch**

10:00 Intermission.

10:20 FLUO 18. Aluminum chlorofluoride–AlF_xCl_y: Fluorine chemist catalyst of choice. **V. Petrov**

10:50 FLUO 19. Fluoride sol-gel procedures: Preparation of some atypical forms of nanostructured fluorides. **T. Skapin**

11:20 FLUO 20. Activation of fluorinated olefins by synergistic action at metal and silicon centres. **T. Braun**, E. Kemnitz, T. Ahrens, C. von Hahmann, C. Xu, G. Meißner, A. Raza, M. Talavera

MONDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Erhard Kemnitz

T. Braun, D.A. Dixon, *Organizers*
S. Riedel, R.G. Syvret, *Presiding*

1:00 FLUO 21. Computational studies of main group and actinide fluorides and new fluoride affinities. **D.A. Dixon**

1:30 FLUO 22. Silver(2+) fluorides: Low dimensional magnetism with extremely strong superexchange. **W. Grochala**

2:00 FLUO 23. Chemistry of uranium and halogen fluorides. **F. Kraus**

2:30 Intermission.

2:50 FLUO 24. Using anhydrous hydrogen chloride as a probe molecule

‡*Cooperative Cosponsorship*

for aluminum fluoride Lewis acids. **J.M. Winfield**

3:20 FLUO 25. Perfluorocarbon-liquids as ophthalmic devices–a piece of cake? **D. Menz**, H. Menz, T. Lechner

3:50 FLUO 26. Award Address (ACS Award for Creative Work in Fluorine Chemistry Sponsored by the ACS Division of Fluorine Chemistry). From crystalline to nanoscopic metal fluorides: A transformation into a different world of materials properties. **E. Kemnitz**

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
N. Vasdev, *Organizer*
8:00–10:00

FLUO 27. Recent advances in the epoxidation of perfluoro- and hydrofluoroolefins. **D.R. Brandt**, V. Petrov

FLUO 28. Synthesis of a heptapeptide containing an optically active trifluoromethyl- β^6-tetrafluorosulfanyl-substituted amino acid. **A. Ikeda**, A.M. Capellan, J.T. Welch

TUESDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Erhard Kemnitz

T. Braun, D.A. Dixon, *Organizers*
I. Krossing, J.T. Welch, *Presiding*

8:00 FLUO 29. Industrial scale fluorochemical synthesis: Importance of liquid- and gas-phase fluorination catalysis for halogen exchange chemistry in the preparation of low global warming potential (GWP) fluorocarbons. **R.G. Syvret**

8:30 FLUO 30. Preparation of new hydrofluoroethers (HFEs) by the addition of tetrafluoroethylene (TFE) to 2,2-dimethyl-1,3-dioxolane and subsequent reactions. X. Liu, M.J. Bulinski, M.G. Costello, **J.S. Thrasher**

9:00 FLUO 31. New fluorinated components for lithium-ion batteries. **G. Roeschenthaler**, I. Cekic-Laskovic, M. Winter

9:30 FLUO 32. Fluorinated compounds synthesis in superacid. T. Cantin, U. Castelli, L. Lebedel, A. Mamontov, B. Michelet, A. Trouiller, H. Carreyre, F. Lecornué, A. Mingot, **S. Thibaudeau**

10:00 Intermission.

10:20 FLUO 33. Mechanochemical synthesis, structure and characterization of fluorine-containing alkaline earth metal compounds **G. Scholz**

10:50 FLUO 34. Theoretical investigations of metal oxofluorides. **B. Paulus**

11:20 FLUO 35. Fluorine-based nanomaterials: what did you expect and what are you expecting. **A. Demourgues**

TUESDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Erhard Kemnitz

T. Braun, D.A. Dixon, *Organizers*
D. Lentz, J.S. Thrasher, *Presiding*

1:00 FLUO 36. New fluorocarbon materials for electronic applications. **O.V. Boltalina**, S.H. Strauss, X. Wang, N.J. DeWeerd, B.J. Reeves, C. Brook

1:30 FLUO 37. When fluorine meets carbon: Reactivity mechanisms, structural changes and applications. **A. Tressaud**, E. Durand, H. Groult

2:00 FLUO 38. Room temperature generation of F_2 gas from $Cs(FH)_{2.45}F$ molten salt. **K. Matsumoto**, T. Sugimoto, T. Inoue, R. Hagiwara

2:30 Intermission.

2:50 FLUO 39. Perfluoroalkylhydridoboranes and -borates: From ionic liquids to Lewis acid-base chemistry. P.T. Hennig, L.N. Schneider, J. Sprenger, N.V. Ignat'ev, **M. Finze**

3:20 FLUO 40. Novel transition metal carbonyl cations: What are the limits with large WCA counterions? **I. Krossing**

3:50 FLUO 41. Hydroarylation of olefins and methane H/D exchange reactions catalyzed by aluminum chlorofluoride (ACF). **B. Calvo**

4:10 Concluding Remarks.

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

Radiopharmaceutical Chemistry
Cosponsored by INOR‡, MEDI‡ and NUCL‡
S.E. Lapi, A.B. Packard, G.D. Tamagnan, N. Vasdev, *Organizers*

6:00–8:00

FLUO 42. Quality control development for the improved clinical production of 3′-deoxy-3′-[^{18}F]fluorothymidine, which utilizes 3-methyl-3-pentanol, for pediatric cancers. **A. Nguyen**, J. Mishra, R. Marino, H. Tillman, B. Kahali, L. Cunningham, E. Butch, S.E. Snyder

FLUO 43. Bio-inspired peptoid chelators for imaging and targeted alpha therapy. **J.A. Rees**, S.J. O'Sullivan, R.J. Abergel

FLUO 44. Synthesis and evaluation of novel hydrophilic molecule for 19F MRI application. **L. Devkota**, C. Ngwa, K.B. Ghaghada, E.A. Tanifum, A.V. Annapragada

WEDNESDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

Radiopharmaceutical Chemistry

Fluorine

Cosponsored by INOR‡, MEDI‡ and NUCL‡
S.E. Lapi, A.B. Packard, *Organizers*
G.D. Tamagnan, N. Vasdev, *Organizers, Presiding*

8:00 FLUO 45. New approaches to radiotrifluoromethylations. **V.W. Pike**

8:30 FLUO 46. Design, synthesis and preliminary evaluation of fluorinated glycogen synthase kinase-3 inhibitors for PET neuroimaging. **V. Bernard-Gauthier**, H. Krishnan, S.H. Liang, N. Vasdev

8:50 FLUO 47. In situ radiosynthesis of L-5-[^{18}F]fluorotryptophan. Y. Xin, **K. Nasr**, X. Sun

9:10 FLUO 48. Radiosynthesis and evaluation of fluorine-18 and carbon-11 radiotracers for PET Imaging of PDE10A in colorectal cancer. **J. Fan**, N. Yasui, B. Kasten, S. Samuel, X. Chen, G. Piazza, Z. Luo, Z. Tu

9:30 Intermission.

9:50 FLUO 49. Re(I) promoted ^{18}F-fluorination reactions for the preparation of PET / optical molecular probes. **B.H. Fraser**, M. Klenner, M. Massi, G. Pascali

10:10 FLUO 50. Transition-metal mediated late-stage radiofluorination. S. Lee, S. Thompson, A. Mossine, N. Ichiishi, I. Jackson, S.W. Krska, M. McCammant, K.J. Makaravage, P. Melvin, M.S. Sanford, P.J. Scott, **A.F. Brooks**

10:30 FLUO 51. Fluorinated peptides and peptidomimetics targeting the ghrelin receptor (GHSR-1a). **L.G. Luyt**

10:50 FLUO 52. Design and radiosynthesis of [^{18}F]dibenzocyclooctynes for highly efficient radiolabelling of macromolecules *via* strain-promoted alkyne-azide cycloaddition. **A. Kostikov**, V. Popik

WEDNESDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

Radiopharmaceutical Chemistry

Carbon-11 & Radionuclide Production

Cosponsored by INOR‡, MEDI‡ and NUCL‡
S.E. Lapi, A.B. Packard, *Organizers*
G.D. Tamagnan, N. Vasdev, *Organizers, Presiding*

1:00 FLUO 53. Carbonylations beyond aryl-X: Development of new multicomponent reactions. **L.R. Odell**, L. Åkerbladh, L. Schembri, P. Nordeman, S. Roslin, J. Eriksson

1:30 FLUO 54. ^{11}C-Carbonylation via "in-loop" $^{11}CO_2$-fixation. **K. Dahl**, T.L. Collier, S.H. Liang, N. Vasdev

1:50 FLUO 55. Strategies for the radiochemical synthesis of ^{11}C-labeled 2- and 3-trifluoromethyl-4-aminopyridine: Potential radioligands for imaging brain demyelination. **P. Brugarolas**, B. Yang, J. Sanchez-Rodriguez, S. Telu, V.W. Pike

2:10 FLUO 56. Expanding the radiochemistry toolbox for PET tracer synthesis. **D. Vugts**

2:40 Intermission.

3:00 FLUO 57. Recent advances in actinium-225 production, chemistry, and applications. **P.D. Benny**, T.R. Dyke, R.A. Boll

3:30 FLUO 58. Production and characterization of titanium-45 for PET imaging. **I.F. Chaple**, A.V. Massicano, B. Wright, E. Boros, S.E. Lapi

3:50 FLUO 59. Auger-emitting ^{119}Te/^{119}Sb production for radiotherapy. **K. Bennett**, S. Bone, J. Engle, S.A. Kozimor

4:20 FLUO 60. Manganese-52 production: Cross-section measurements via irradiation of natural chromium targets. **R. El Sayed**, A.V. Massicano, S.E. Lapi

THURSDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

Radiopharmaceutical Chemistry
Cosponsored by INOR‡, MEDI‡ and NUCL‡
G.D. Tamagnan, N. Vasdev, *Organizers*
S.E. Lapi, A.B. Packard, *Organizers, Presiding*

8:00 FLUO 61. Zr-89 based multimodal probes. **E. Boros**

8:30 FLUO 62. Influence of chelator conjugation method on immunoPET imaging. **D. Vivier**, C. Rodriguez, P. Adumeau, B. Zeglis

8:50 FLUO 63. Inorganic ion-exchangers for radiochemical separations of Y/Zr and Sc/Ti. **S.L. Queern**, C.L. Manderbach, C.S. Cutler, D.G. Medvedev, S.E. Lapi, J.M. Fitzsimmons

9:10 FLUO 64. ImmunoPET imaging of the soluble protein interferon-β. **N. Viola-Villegas**, H. Gibson, B. McKnight, W. Wei

9:40 Intermission.

10:00 FLUO 65. Direct astatination of poly(adenosine diphosphate ribose) polymerase inhibitors using boronic acid precursors. **M. Makvandi**, S.W. Reilly, R.H. Mach

10:30 FLUO 66. Production of theranostic radioscandium for nuclear imaging and radiotherapy. **C.S. Loveless**, G.L. Diehl III, L.L. Radford, S.E. Lapi

10:50 FLUO 67. Spectroscopic studies of actinium coordination chemistry. **B.W. Stein**, M.G. Ferrier, S.A. Kozimor, E.R. Batista, J.M. Berg, E.R. Birnbaum, K.D. John, P. Yang

THURSDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 1/2

Radiopharmaceutical Chemistry
Cosponsored by INOR‡, MEDI‡ and NUCL‡
G.D. Tamagnan, N. Vasdev, *Organizers*
S.E. Lapi, A.B. Packard, *Organizers, Presiding*

1:00 FLUO 68. New ^{55}Co PET-agent as a diagnostic analog for ^{153}Sm-DOTMP. **L.L. Radford**, S. Ellebracht, L. Swirsky,

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S. Bright, R. Beacham, R. Frank, J. Simon, S.E. Lapi

1:20 FLUO 69. SPECT/CT imaging of ^{177}Lu-labeled phosphoramidate-based PSMA inhibitor with an albumin-binding motif. **X. Ling**, C.J. Choy, J.D. Latoche, J.J. Geruntho, Y. Wu, N. Salamacha, B. Langton-Webster, C.J. Anderson, C.E. Berkman

1:40 FLUO 70. Synthesis of ^{212}Pb-RM2: A potential radiotherapeutic agent for prostate cancer. **N.C. Okoye**, T. Rold, A. Berendzen, S.S. Jurisson, T.J. Hoffman

2:00 FLUO 71. The development of ^{72,77}As radiopharmaceuticals for potential PET imaging and therapy: production, radiochemistry and biological evaluation. **Y. Feng**, T.E. Phelps, M.D. Phipps, A.J. DeGraffenreid, A.L. Wooten, N. Okoye, A. Ketring, C.S. Cutler, D.S. Wilbur, T.J. Hoffman, S.S. Jurisson

2:20 Intermission.

2:40 FLUO 72. Synthesis and *in vivo* characterization of a ^{68}Ga/NIR labeled peptide for somatostatin receptor targeting. S.C. Ghosh, S. Hernandez Vargas, J. Voss, K. Carmon, **A. Azhdarinia**

3:10 FLUO 73. NOTA and NODAGA ^{99m}Tc/^{186}Re-tricarbonyl complexes: Radiochemistry of model complexes and *in vivo* evaluation of a ^{99m}Tc-NODAGA-SSTR antagonist bioconjugate. **G. Makris**, L.L. Radford, M. Kuchuk, F. Gallazzi, S.S. Jurisson, C.J. Smith, H.M. Hennkens

3:30 FLUO 74. Synthesis and evaluation of MAMA-based bifunctional chelators for the oxorhenium (V) core **F. Najafi Khosroshahi**, D.W. Demoin, A. Dame, Y. Feng, S.S. Jurisson

3:50 FLUO 75. ^{68}Ga-labeled tracer for pretargeted immunoPET imaging of colorectal cancer. **P. Adumeau**, M. Davydova, B. Zeglis

GEOC

Division of Geochemistry

W. Burgos, *Program Chair*

SOCIAL EVENTS:

GEOC Social Hour, 6:00 PM: Tue

BUSINESS MEETINGS:

GEOC Board Meeting, 6:00 PM: Sun

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 355

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Cosponsored by COLL, ENFL, ENVR and INOR
N. Kabengi, M.L. Machesky, A. Navrotsky, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 1. Structure and dynamics of earth materials, interfaces and reactions. **D. Cole**, D. Wesolowski

9:05 GEOC 2. Dave, Don, Moira, me and the HECC. **M.L. Machesky**

9:35 GEOC 3. Complexity at the oxide-water Interface: A clarity of vision. **P. Fenter**

10:05 GEOC 4. S(t)imulating collaboration with Dave Wesolowski: From β (rutile) to β (potential). **M. Predota**, M.L. Machesky, D. Wesolowski, P.T. Cummings

10:35 GEOC 5. Thermodynamic analysis of adsorption and exchange of alkali metal cations on rutile. **P. Ilani Kashkouli**, L. Wu, N. Kabengi, A. Navrotsky

10:55 Intermission .

11:05 GEOC 6. Atomic- to pore-scale geochemistry: Effects of ion sorption and incorporation on mineral growth. **A.G. Stack**, A. Bertagni, J. Bracco, M. Cheshire, C. Dai, N. Deng, P. Fenter, S.R. Higgins, Y. Hu, A. Ievlev, S. Jindra, J.D. Kubicki, S. Lee, M. Lorenz, K. More, V. Starchenko, J. Weber

11:35 GEOC 7. Relationship between incorporation of impurity cations and their effects on mineral growth: High-resolution in- and ex-situ observations in the (Ba,Sr)SO_4 system. **J. Weber**, J. Bracco, S.R. Higgins, K. More, M. Lorenz, A. Ievlev, J.D. Poplawsky, S. Jindra, A.L. Bertagni, A.G. Stack

11:55 GEOC 8. Effects of strontium impurity on barite precipitation in mesoporous media. **V. Starchenko**, M. Cheshire, J. Weber, A.G. Stack

12:15 Discussion.

Section B
Ernest N. Morial Convention Center
Room 338

Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes
Cosponsored by AGRO and ENVR
M. Keiluweit, *Organizer*
N. Senesi, B. Xing, Y. Yang, *Organizers, Presiding*
M. Keiluweit, *Presiding*

8:30 Introductory Remarks.

8:35 GEOC 9. Geochemical and mathematical constraints on the carbon sequestration potential of eroding watersheds. **A. Berhe**, T.A. Ghezzehei

9:05 GEOC 10. Ferrous iron oxidation under varying pO_2 levels: The effect of Fe(III)/Al(III) oxide minerals and organic matter. C. Chen, **A. Thompson**

9:35 GEOC 11. Transport and Transformation of Particulate Organic Matter in Permeable Riverbed Sediments. S. Bessey, J. Mejia, N. Stern, S. Loheide, E.E. Roden, **M.A. Ginder-Vogel**

9:55 GEOC 12. Iron electron transfer and atom exchange in ferrihydrite-NOM Co-precipitates. **Z. Zhou**, D. Latta, N. Noor, A. Thompson, M. Scherer

10:15 Intermission.

10:30 GEOC 13. Multi-scale dynamics of carbon cycling in orchards as a function of irrigation type. C. Avila, M.V. Schaefer, N. Bogie, E. Dubinsky, E. Brodie, M. Fogel, A. Marklein, D. Rath, A. Berhe, T.A. Ghezzehei, S.J. Parikh, W. Riley, K. Scow, M. Torn, **S. Ying**

11:00 GEOC 14. Characterization and phenanthrene sorption of natural and pyrogenic organic matter fractions. **K. Sun**, J. Jin, B. Xing

11:30 GEOC 15. Aerobic microbial respiration of mineral-bound organic carbon: Bioavailability and priming effects. **D. Adhikari**, D. Wordofa, S. Dunham-Cheatham, S. Poulson, E.E. Roden, Y. Yang

11:50 GEOC 16. Adsorption and molecular fractionation of dissolved organic matter on iron-bearing mineral matrices of varying crystallinity. **E.K. Coward**, T. Ohno, A.F. Plante, D.L. Sparks

12:10 GEOC 17. Humic-like products formation via the reaction of phenol with nitrite in ice phase. **D. Min**, W. Choi

Section C
Ernest N. Morial Convention Center
Room 339

Biomineralization & Bio-Compatible Minerals
Cosponsored by BIOL and ENVR
J.D. Rimer, *Organizer*
J.A. Soltis, G. Zhu, *Organizers, Presiding*

9:00 Introductory Remarks.

9:00 GEOC 18. Understanding the mechanisms of biomineralisation: a grand challenge. **J. Harding**, C. Freeman, A. Finney, R. Innocenti Malini

9:30 GEOC 19. Nucleation and growth of crystalline carbonates from amorphous precursors. **D. Joester**

10:00 GEOC 20. How corals build reefs from nanoparticles. **P. Gilbert**

10:30 Intermission.

10:50 GEOC 21. Elucidating the intracellular chemical environment that regulates biological calcite crystallization in marine plankton. **A. Gal**, J. Mahamid, D. Faivre, A. Scheffel

11:20 GEOC 22. Uptake of uranium by plants in waters containing calcium and carbonate. **E. El Hayek**, C. Torres, L. Rodriguez Freire, A. Brearley, M. Spilde, S. Cabaniss, A. Ali, J.M. Cerrato

11:40 GEOC 23. Thermodynamics of confined calcium phosphate nucleation in collagen fibrils. **D. Kim**, B. Lee, S. Thomopoulos, Y. Jun

12:00 GEOC 24. Structure flexibility controls the adsorption and digestion kinetics of point mutant amelogenin on hydroxyapatite (100). **J. Tao**, R. Jayasinha Arachchige, B. Tarasevich, Y. Shin, G. Buchko, W. Shaw, J. De Yoreo

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Energy, Water & Food Production
Sponsored by AGFD, Cosponsored by CELL, GEOC and MPPG

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 355

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Cosponsored by COLL, ENFL, ENVR and INOR
N. Kabengi, M.L. Machesky, A. Navrotsky, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 GEOC 25. A decade modeling the mineral-water interface: Is there an electrical double layer? **J.D. Kubicki**

2:05 GEOC 26. Molecular simulation of ionic liquids at interfaces: Effects of solvation, humidification, and mixing. **M.W. Thompson**, N.C. Osti, K. Van Aken, B. Dyatkin, F. Tiet, R. Matsumoto, E. Mamontov, Y. Gogotsi, P.T. Cummings

2:25 GEOC 27. Electrical double layer in nanoporous electrodes. **J. Wu**

2:45 GEOC 28. Atomistic structure of mineral nano-aggregates from simulated compaction and dewatering. **L.J. Criscenti**, T.A. Ho, J.A. Greathouse, Y. Wang

3:05 Intermission.

3:20 GEOC 29. Not to be soon revised—Dave Wesolowski's accomplishments in understanding hydrothermal chemistry. **W.H. Casey**

3:50 GEOC 30. David Wesolowski's contributions to hydrothermal geochemistry. **H. Ohmoto**

4:20 GEOC 31. Hydrothermal synthesis of chromian spinel from iron and chromium hydroxides using a flow-through apparatus. **T. Otake**, M. Nishikata, Y. Ohtomo, Y. Kimura, D. Kawamoto, T. Sato

4:40 GEOC 32. Nonlinear surface spectroscopy of the β-quartz/water interface. **F. Geiger**

5:00 GEOC 33. A setup for combined zeta-potential and second harmonic generation measurements. **J. Luetzenkirchen**

5:20 Discussion.

Section B
Ernest N. Morial Convention Center
Room 338

Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes
Cosponsored by AGRO and ENVR
M. Keiluweit, *Organizer*
N. Senesi, B. Xing, Y. Yang, *Organizers, Presiding*
M. Keiluweit, *Presiding*

1:30 GEOC 34. Influence of soil carbon and priming effects on greenhouse gases emissions in degraded wetlands restored with rice cultivation. **W. Horwath**, R. Ye, J. Morris

2:00 GEOC 35. Microbial physiology and products drive soil organo-mineral interactions and bioavailable nitrogen dynamics. **S. Grandy**, C. Kallenbach, A. Jilling

‡*Cooperative Cosponsorship*

2:30 GEOC 36. Molecular characterizations of soil carbon responses to nitrogen additions. **Q. Zhao**, K. Hofmockel, M. Tfaily, S. Callister, R. Kukkadapu, L. Bramer

2:50 GEOC 37. Synergistic effect of calcium on organic carbon sequestration to ferrihydrite: Potential for Fe-Ca-OC ternary complexes. **T.D. Sowers**, J. Stuckey, D. Adhikari, Y. Yang, D.L. Sparks

3:10 Intermission.

3:30 GEOC 38. Interconnecting soil organic matter with N and P cycling. **L. Celi**

4:00 GEOC 39. Linking sources and transformation of phosphorus in the soil-water continuum in the estuarine environment. **D. Jaisi**, M. Sun, S. Joshi, L. Stout, K. Bear

4:30 GEOC 40. Phosphorus speciation in atmospherically deposited air particulates from high and low elevation sites of California and Colorado. **U.G. Nwosu**, B. Lash, M. Barnes, S.C. Hart, A. Berhe, P.A. O'Day

4:50 GEOC 41. Investigation of carbon cycling in a subtropical estuary subjected to an early-season flood pulse, and secondary sources. **B.J. Haywood**, J.R. White, R.L. Cook

5:10 GEOC 42. Impact of redox reactions on carbon stability: Reduction, oxidation, and reduction-oxidation transition. D. Adhikari, Q. Zhao, K.K. Das, X. Wang, S. Poulson, Y. Tang, D. Obrist, E.E. Roden, **Y. Yang**

Section C
Ernest N. Morial Convention Center
Room 339

Biomineralization & Bio-Compatible Minerals
Cosponsored by BIOL and ENVR
J.D. Rimer, *Organizer*
J.A. Soltis, G. Zhu, *Organizers, Presiding*

1:30 GEOC 43. 3D breast tumor model for studying the formation mechanisms of microcalcifications. **N. Vidavsky**, J.A. Kunitake, C. Fischbach, L.A. Estroff

2:00 GEOC 44. Influence of structural defects on biomineralized ZnS nanoparticle dissolution: An in-situ electron microscopy study. J. Eskelsen, J. Xu, M. Chiu, J. Moon, B. Wilkins, D.E. Graham, B. Gu, **E. Pierce**

2:20 GEOC 45. Biomineralization of metals in bacterial organelles. C. Grant, L. Rahn-Lee, M. Byrne, **A. Komeili**

2:50 Intermission.

3:10 GEOC 46. Role of amelogenin β-sheet ribbons in biomineralization of hydroxyapatite. **S. Akkineni**, S. Engelberth, J. Tao, J. Bonde, S. Habelitz, J.J. DeYoreo

3:30 GEOC 47. Self-organization of biomimetic polycrystalline precursors into fractals. **P. Knoll**, O. Steinbock

Carbon Dioxide Conversion & Artificial Photosynthesis
Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Energy, Water & Food Production
Sponsored by AGFD, Cosponsored by CELL, GEOC and MPPG

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 338

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Cosponsored by COLL, ENFL, ENVR and INOR
N. Kabengi, M.L. Machesky, A. Navrotsky, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 48. Geochemistry and materials science teach each other: A tribute to "Weso". **A. Navrotsky**

9:05 GEOC 49. Fluid interface reactions, structures and transport. D. Wesolowski, **Y. Gogotsi**

9:35 GEOC 50. Two-dimensional transition metal carbides and nitirdies, MXenes, as host materials for ions. **M. Naguib**, H. Wang, N.C. Osti, A.I. Kolesnikov, L. Vlcek, E. Mamontov, P. Kent

9:55 GEOC 51. Molecular simulations of fluid-solid interfaces around hydrated clay particle edges and site-specific adsorption of divalent cations at these surfaces. **B.F. Ngouana-Wakou**, I. Androniuk, A.G. Kalinichev

10:15 GEOC 52. Dynamical restructuring of bi-Ionic liquid solution interfaces during electrochemical CO_2 reduction. **J. Medina Ramos**, S. Lee, A. Hubaud, T. Fister, P. Fenter

10:35 Intermission.

10:50 GEOC 53. Effects of phosphonates on physicochemical properties of mica under energy-related subsurface conditions. **L. Zhang**, Y. Jun

11:10 GEOC 54. Improving nucleation predictions through understanding of ion-water and ion-ion interactions in concentrated solutions. **H. Wang**, L. Vlcek, K. Page, J. Neuefeind, A.G. Stack

11:30 GEOC 55. Thermodynamic properties of water confined on metal oxide nanoparticles using inelastic neutron scattering. **N.L. Ross**, A.I. Kolesnikov, B.F. Woodfield, A. Navrotsky

11:50 GEOC 56. Fluid-solid interfacial phenomena at the nexus of energy and geochemistry research. **D. Wesolowski**

Section B
Ernest N. Morial Convention Center
Room 355

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Cosponsored by ENVR
M.B. Hay, D.B. Kent, *Organizers*
K. Campbell, *Organizer, Presiding*
S.P. Hyun, *Presiding*

8:30 Introductory Remarks.

8:40 GEOC 57. Quantum calculations modeling arsenic and uranium adsorption. **J.D. Kubicki**

9:00 GEOC 58. The MUSE: A multi–start optimization algorithm for surface complexation parameters in complex systems. **M. Chrysochoou**, N. Bompoti, M.L. Machesky

9:15 GEOC 59. Modeling uranium(VI) adsorption onto montmorillonite under varying carbonate concentrations: A surface complexation model accounting for the spillover effect on surface potential. **C. Tournassat**, R.M. Tinnacher, S. Grangeon, J.A. Davis

9:30 GEOC 60. Intercomparison of surface complexation models for uranium(VI) adsorption to goethite: Sources of variation in model output and movement toward a more globally optimal model. **A. Satpathy**, D. Giammar

9:45 GEOC 61. Surface complexation modeling – From BSM back to TLM?. **J. Luetzenkirchen**

10:00 GEOC 62. Biogeochemical interfacial reactivity in a changing environment. **D.L. Sparks**

10:25 Intermission.

10:50 GEOC 63. Effects of fulvic acid on uranium(VI) sorption kinetics: Using kinetics to characterize metal sorption processes. **R.M. Tinnacher**, P.S. Nico, J.A. Davis, B. Honeyman

11:10 GEOC 64. Assessing the need for complexity in surface complexation models of goethite. L.E. Katz, **J. Han**

11:25 GEOC 65. U(VI) and Fe-containing oxyhydroxide and clay minerals: Redox reactivity and products. **M. Boyanov**, D. Latta, B. Mishra, M. Scherer, S. Yan, E.J. O'Loughlin, K.M. Kemner

11:40 GEOC 66. A mean electrostatic model for ion transport through heterogeneous clay. **C. Steefel**, C. Tournassat

11:55 GEOC 67. Effect of Long-Term Bentonite Heating on U(VI) Adsorption. **P. Fox**, P.S. Nico

12:10 GEOC 68. Surface complexation from the grain to plume scale in a gravel aquifer influenced by groundwater–surface water exchange: Considerations for system predictability. **J. Zachara**, X. Chen, D.B. Kent, C. Liu

Section C
Ernest N. Morial Convention Center
Room 339

Contaminated Site Remediation through Microbial, Geological & Chemical Processes
Cosponsored by ENVR
B. Jeon, Y. Ok, D. Tsang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 69. Modeling framework for adsorption processes in environmental remediation and monitoring. A. Ladshaw, C. Tsouris, **S. Yiacoumi**

9:05 GEOC 70. Exploring the mechanisms of trace metals immobilization by biochar. **D. Alessi**

9:35 GEOC 71. Testing the feasibility of temperature monitoring to determine degradation rates at a crude oil spill site. **E. Warren**, B.A. Bekins

9:55 GEOC 72. Contributions of abiotic, aerobic pathways to chlorinated ethene degradation during back diffusion from low permeability zones. **E. Berns**, A. Valocchi, R. Sanford, T.J. Strathmann, C. Schaefer, C.J. Werth

10:15 Intermission.

10:35 GEOC 73. Effects of temperature on aggregation, retention, and transport of graphene oxides in granular porous media. **B. Gao**, M. Wang

11:05 GEOC 74. Assessment and remediation of arsenic-containing soils for urban development in Hong Kong. **D. Tsang**, C.S. Poon, X. Li

11:25 GEOC 75. Nanoscale examinations on the speciation of copper within organic matter from soils contaminated by mining activities. **H. Mantha**, M. Schindler, M.F. Hochella

11:45 GEOC 76. Using flow-through columns to optimize the microbially-driven Fenton reaction for the in situ degradation of organic contaminants. **N. Xie**, Y.J. Toporek, T.J. Dichristina, M. Taillefert

12:05 GEOC 77. Effect of heating time and peak temperature of pyrolysis on biochar derived from rice husk. **S. Chandra**, J. Bhattacharya

Carbon Dioxide Conversion & Artificial Photosynthesis

Theoretical Studies, Policy & Catalytic Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 338

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Cosponsored by BIOL and ENVR
W.D. Burgos, C. Chan, S. Crowe, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 GEOC 78. Stable isotope insights into redox connections in the cycling of nitrogen and metals. **S.D. Wankel**

2:05 GEOC 79. Microbially mediated nitrate-reducing Fe(II) oxidation: Quantification of chemodenitrification and enzymatic reactions. **T. Liu**, D. Chen, X. Luo, F. Li

2:35 GEOC 80. Influence of inter-species competition on the kinetics and extent of microbial anaerobic Fe(II) oxidation. **C. Bryce**, L. Sauter, Y. Huang, S. Kleindienst, A. Kappler

3:05 Intermission.

3:30 GEOC 81. Oxidative extracellular electron transfer–rethinking the role of microbes in biogeochemical cycles. **A. Bose**

4:00 GEOC 82. Evaluation of microbially-induced carbon steel corrosion using zero resistance ammetry in a split-chamber format. **J.M. Senko**, R.B. Miller, C. Monty, A. Sadek

4:30 GEOC 83. Geochemical and temporal influences on the enrichment of acidophilic iron-oxidizing bacterial communities. **W.D. Burgos**

Section B
Ernest N. Morial Convention Center

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Room 355

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Cosponsored by ENVR
K. Campbell, D.B. Kent, *Organizers*
M.B. Hay, *Organizer, Presiding*
J. Luetzenkirchen, *Presiding*

1:30 Introductory Remarks.

1:35 GEOC 84. Elemental partitioning between aqueous and solid phases that form in wastewater brine from a shale-gas well evolves during storage prior to disposal. **D.B. Kent**, M. Marvin-DiPasquale, M. Engle, M.S. Blondes, C. Conaway, W.H. Orem, I.M. Cozzarelli, J.B. Jaeschke, M. Kohler, M.R. Arias, L. Kieu, M. Mnich, K.J. Skalak, M.S. Varonka

1:50 GEOC 85. Constituent ions and "spectator" low molecular weight organic acids influence ligand exchange kinetics: Geochemical implications. **N.E. Boland**, A.T. Stone, A. Wildman, Y. Xu, L. Rea, E. Briody-Pavlik, Z. Huang

2:05 GEOC 86. Investigation on Pb-calcite interaction by transmission X-ray microscopy. **K. Yuan**, S. Lee, V.D. Andrade, N.C. Sturchio, P. Fenter

2:20 GEOC 87. Cadmium removal mechanism by mackinawite under anoxic conditions. **S.P. Hyun**, B. Kim, K.F. Hayes

2:35 GEOC 88. Arsenate sorption on iron oxyhydroxides: Initial studies with James A. Davis and updated analysis. **G.A. Waychunas**

2:55 GEOC 89. Interfacial geochemistry in practice: Arsenic and household water treatment. **J. Hering**

3:20 Intermission.

3:45 GEOC 90. Arsenic mobilization and attenuation during injection of treated coal seam gas co-produced water into deep aquifers. B. Rathi, A. Siade, M. Donn, L. Helm, R. Morris, J.A. Davis, M. Berg, **H. Prommer**

4:00 GEOC 91. Geochemical processes along hyporheic redox gradients controlling carbon and metal transformations. **P.S. Nico**, J.A. Davis, X. Yuan

4:15 GEOC 92. Control of U(IV) transformation and mobilization by nano-scale FeS_{x-1} in suboxic and oxic systems. **Y. Bi**, K.F. Hayes

4:35 GEOC 93. Microbially-mediated metal/radionuclide oxidation coupled to nitrate reduction in an alluvial aquifer. **K. Weber**, J. Westrop, J. Nolan, S. Bone, J.R. Bargar, K. Campbell, D.D. Snow

4:55 GEOC 94. The stability of non-crystalline U(IV) under oxic and anoxic conditions. **R. Bernier-Latmani**, L. Loreggian, S. Bretagne, A. Novotny

5:15 GEOC 95. Post audit of a reactive transport model of hexavalent uranium migration in a shallow alluvial aquifer. **G.P. Curtis**, M. Kohler

Section C
Ernest N. Morial Convention Center
Room 339

Contaminated Site Remediation through Microbial, Geological & Chemical Processes
Cosponsored by ENVR
B. Jeon, Y. Ok, D. Tsang, *Organizers, Presiding*

1:30 GEOC 96. Gasification-derived biochar adsorbents for wastewater treatment and emerging contaminants removal. T. Maneerung, W. Ng, X. Cui, **C. Wang**

2:00 GEOC 97. From environmental biotechnology research to continued application: The challenges and roadblocks to address. **J. Bhattacharya**

2:25 GEOC 98. Electron doping of iron minerals by dissolved sulfide: Implications for contaminant reduction. **D. Latta**, T. Robinson, J. Entwistle, A. Neumann, Y. Lan, M. Bradley, P.G. Tratnyek, M. Scherer

2:45 GEOC 99. Valorization of sewage sludge for attenuation of polycyclic aromatic hydrocarbons (PAHs) in simulated crude oil contaminated soil. **N.O. Offiong**, **E.J. Inam**

3:05 GEOC 100. Synthesis of novel adsorbent β-cyclodextrin-graphene oxide nanocomposite (β-CD-GO) for the potentially enhanced removal of dyes and heavy metals from wastewater. **R. Rathour**, J. Bhattacharya

3:25 Intermission.

3:40 GEOC 101. Degradation of the perchlorate anion through chemical and electrochemical methods. **K. Paeng**, E. Kim, H. Jee, N. Myung

4:05 GEOC 102. Synthesis and characterization of hydrochars with PHC sorption properties. **D. Bulmer**, P. Mussone, S. Siciliano, D. Peak

4:25 GEOC 103. Structural variability in manganese oxides produced at a coal mine drainage remediation site. **M.A. Hinkle**, F.T. Ling, P. Heaney, J. Post

4:45 GEOC 104. PCB dechlorination hotspots and reductive dehalogenase genes in sediments from a contaminated wastewater lagoon. **J.M. Ewald**, Y. Liang, A. Martinez, A. Awad, J.L. Schnoor, K.C. Hornbuckle, T. Mattes

5:05 GEOC 105. Methanol self-association and preferential solvation of chelating agents for the extraction of heavy metals in sCO_2. **T. Graham**, D. Pope, Y. Ghaadrghadr, S.B. Clark, A.E. Clark, S.R. Saunders

5:25 Concluding Remarks.

Carbon Dioxide Conversion & Artificial Photosynthesis
Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Redox & Interfacial Dynamics Among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients
Sponsored by ENVR, Cosponsored by GEOC

Undergraduate Research Posters

Geochemistry

Sponsored by CHED, Cosponsored by GEOC and SOCED

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 355

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Cosponsored by BIOL and ENVR
W.D. Burgos, C. Chan, S. Crowe, *Organizers, Presiding*

9:00 GEOC 106. Thiols as proxies for the biogeochemical transformation of iron, manganese, and sulfur in marine sediments. **M. Taillefert**, E. Eitel, A. Bertagnolli, A. Burns, F. Stewart, T.J. Dichristina

9:30 GEOC 107. Relevance of stratified Midwestern lakes to past, present, and future microbial biogeochemistry. **E.D. Swanner**, C. Wittkop, S. Katsev, N. Lambrecht, M. Fakhraee

10:00 GEOC 108. Redox regime shifts in euxinic marine environment (Rogoznica Lake, eastern Adriatic coast). **I. Ciglenecki**, M. Margus, M. Cankovic, A. Cvitesic, I. Petric, G. Collins, N. Mikac

10:30 Intermission.

10:50 GEOC 109. Characterizing and solving environmental arsenic contamination through combined geochemical, geobiological and organic matter characterization. **B.C. Bostick**, J. Sun, A. Nghiem, J. Jamieson, H. Prommer, B. Yan, L. van Geen, B. Mailloux, S. Chillrud

11:20 GEOC 110. Investigating the relationship between mercury methylation and microbial community composition across sulfate gradients in Northern Minnesota. **D.S. Jones**, N.W. Johnson, C. Mitchell, G. Walker, J.K. Coleman Wasik, E.B. Swain, J.V. Bailey

11:50 GEOC 111. Effects of minerals on mercury methylation by *Desulfovibrio desulfuricans* ND132. **L. Zhao**, S. Wu, X. Lu, H. Chen, B. Gu

12:10 GEOC 112. Modeling the kinetics of bacterial metal bioavailability: The role of metal adsorption. **J. Fein**

Section B
Ernest N. Morial Convention Center
Room 338

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Cosponsored by ENVR
K. Campbell, M.B. Hay, D.B. Kent, *Organizers*
A. Amirbahman, H. Prommer, *Presiding*

8:30 GEOC 113. Surface catalyzed carbonate and bicarbonate reduction: Implications on serpentinization-related abiotic methane production. **Y. He**, J. Wang, H. Bao

8:45 GEOC 114. Introducing soft X-ray based excitation emission matrix spectroscopy for geochemical analysis. **D. Peak**, J. Hamilton, T.Z. Regier

9:00 GEOC 115. Synthesis of engineered soil surrogates. **A. Pandey**, G. Abdalla, B.J. Haywood, S.P. Smith, B. Subramanian, R.L. Cook, D. Spivak

9:15 GEOC 116. Mechanisms of tripolyphosphate adsorption and hydrolysis on mineral surfaces. **J. Hamilton**, D. Peak

9:30 GEOC 117. Flume simulations of Fe oxidation and deposition in abandoned mine drainage. W.A. Peterson, E.K. Herman, **M.M. McGuire**

9:45 GEOC 118. The relationship between hydro-geomorphic setting and geochemical gradients along flowpaths in stream sediments impacted by acid mine drainage. **D. Singer**, A.J. Jefferson, E.L. Traub, N. Perdrial

10:00 GEOC 119. Controls on phosphorus export from an agricultural watershed with calcareous bedrock and surficial geology. G. McDonald, **A. Amirbahman**, S. Norton, I. Fernandez, K. Hoppe, J. Dennis

10:15 Intermission.

10:30 GEOC 120. Nano-environmental science as an emerging field, with a tribute to Jim Davis and his enduring legacy. **M.F. Hochella**

10:55 GEOC 121. Uranium uptake and redistribution in iron oxide nanoparticles: Effects of phase transformation and crystal growth mechanism. **J.A. Soltis**, M.E. McBriarty, S. Spurgeon, J.J. DeYoreo, E. Ilton

11:10 GEOC 122. Role of iron in controlling radionuclide migration at a legacy waste site exhibiting dynamic redox transitions. **D. Waite**, T. Payne, A. Kinsela, M. Bligh, X. Vazquez-Campos

11:30 GEOC 123. Oxidative uranium release from anoxic sediments under diffusion-limited conditions. **S. Bone**, M.R. Cahill, M.E. Jones, S.E. Fendorf, J.A. Davis, K. Williams, J.R. Bargar

11:45 GEOC 124. Vertical transport of uranium in the unsaturated zone: A likely plume persistence mechanism. S. Roycroft, V. Noel, K. Boye, R. Johnson, W. Dam, S.E. Fendorf, **J.R. Bargar**

12:05 GEOC 125. Challenges and advances in translating aqueous geochemistry to bioavailability and toxicity. **S.N. Luoma**

12:25 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 339

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Cosponsored by AGFD, AGRO and ENVR
D. Alessi, T. Borch, N.R. Warner, *Organizers, Presiding*

9:00 GEOC 126. Mining, reclamation, plant productivity, and livestock production implications. **J. Ippolito**

9:30 GEOC 127. Understanding coupled biogeochemical and mineralogical processes that control trace-metal fate in acidic mine water supports water treatment at Iron Mountain Mine, CA. **K. Campbell**, C. Alpers, K. Nordstrom

10:00 GEOC 128. Transport of uranium and co-occurring constituents in abandoned mines in Native American communities. **J.M. Cerrato**, S. Avasarala, A. Ali, J.M. Blake, K. Artyushkova, L. Rodriguez-Freire, C. Velasco, A. Brearley, E. El Hayek

‡*Cooperative Cosponsorship*

10:30 GEOC 129. Speciation and reactivity of uranium and organic matter in abandoned mine wastes from Laguna–New Mexico. **C. Velasco**, S. Avasara, A. Ali, K. Artyushkova, C. Osburn, J.M. Cerrato

10:50 Intermission.

11:10 GEOC 130. Arsenic mobility and reactivity near abandoned mine wastes in Cheyenne River, South Dakota (CRST). **C. DeVore**, L. Rodriguez-Freire, A. Ali, K. Artyushkova, J.M. Cerrato

11:30 GEOC 131. Concurrent removal of boron and scale-forming cations by co-precipitation, adsorption and polymer-enhanced ultrafiltration. **O. Dollar**, E.F. Peltier, M. Chen, K. Shafer-Peltier, S. Randtke

11:50 GEOC 132. Reactive transport modeling of remedial actions at the Pennsylvania Mine near Keystone, Colorado. **R.L. Runkel**, P.L. Verplanck, E. Petri, K. Walton-Day

Carbon Dioxide Conversion & Artificial Photosynthesis

Photocatalytic Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Redox & Interfacial Dynamics Among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients
Sponsored by ENVR, Cosponsored by GEOC

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 355

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Cosponsored by BIOL and ENVR
W.D. Burgos, C. Chan, S. Crowe, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 GEOC 133. Life through the proterozoic. **P. Crockford**

2:05 GEOC 134. Exploring the relative importance of surficial cyanobacteria communities versus physical, chemical and bioloigical processes at depth on sulfur cycling in two microbial mat environments. **M. Gomes**, D. Fike, J. Klatt, U. Lingappa, S. O'Reilly, L. Riedman, S. Grim, K. Metcalfe, G. Dick, W. Fischer, J. Grotzinger, A. Knoll

2:35 GEOC 135. Quantitative indicators of sulfate reducer metabolic state: Isotopes and proteomics. **W.D. Leavitt**, J. Waldbauer, S. Venceslau, M. Sim, A. Bradley

3:05 GEOC 136. Biogeochemical rates in a dark sulfuretum. **J. Macalady**, M. Mansor, B. Kamermans, M.S. Fantle, J. Cosmidis

3:35 Intermission.

4:00 GEOC 137. Shaping the kinetics of methanogenic communities: A multi-omic approach to study interspecies cooperation. **R. Ziels**, H. Stensel, D. Beck

4:30 GEOC 138. Interplay between microbial signatures and mineral precipitation in a geological evaporite. **A. Olcott Marshall**, D. Lockamy

5:00 GEOC 139. Microbial lipid biomarkers in a Marcellus Shale natural gas well: From remnant molecules to adapted communities. **A. Hanson**, J. Lipp, K. Hinrichs, P. Mouser

Section B
Ernest N. Morial Convention Center
Room 338

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Silica/Alumina Surfaces & the Electrical Double Layer

Cosponsored by ENVR and INOR
J. Bracco, S.E. Mason, J. Weber, *Organizers, Presiding*

1:30 GEOC 140. Calorimetry, spectroscopy and density functional theory: Oxyanions and ferrihydrite. **J.D. Kubicki**, N. Kabengi, A. Namayandeh, M. Chrysochoou

2:00 GEOC 141. Comparison of X-ray reflectivity and *ab initio* molecular dynamics structures of the corundum-water and graphene-electrolyte interfaces. **K. Harmon**, K. Letchworth-Weaver, E.J. Bylaska, A. Gaiduk, F. Giberti, S. Lee, T. Fister, J. Weare, M.J. Bedzyk, G.A. Galli, M. Chan, P. Fenter

2:20 GEOC 142. Hydrophobic aqueous interfaces by DFT-MD simulations and vSFG: 2-dimentional H-bond networks. **S. Pezzotti**, A. Serva, D. Galimberti, M.P. Gaigeot

2:40 GEOC 143. Adsorption of oxalic acid on rutile surfaces. D. Biriukov, **M. Predota**, O. Kroutil, M.K. Ridley, M.L. Machesky

3:00 GEOC 144. An *ab initio* study of water at interfaces: The case of alumina adsorbent. **A. Abbaspour Tamijani**, I. Metz, **S.E. Mason**

3:20 GEOC 145. Modeling aluminum nanoclusters in variable chemical environments with first-principles DFT and thermodynamics. **J.L. Bjorklund**, J.W. Bennett, T. Forbes, S.E. Mason

3:40 Intermission.

4:00 GEOC 146. Mineral/water interfaces characterized by Ab initio molecular dynamics: Making the link between structure and SFG vibrational spectroscopy. **M.P. Gaigeot**

4:30 GEOC 147. Relative permittivity in the electrical double layer from nonlinear optics. **F. Geiger**

4:50 GEOC 148. vSFG signals at charged mineral-water interfaces: $\beta^{(3)}$ (β) contributions and how to use them for unraveling interfacial structures. **D. Galimberti**, S. Pezzotti, M.P. Gaigeot

5:10 GEOC 149. Structure of the amorphous colloidal silica-aqueous electrolyte interface: Electrolyte concentration dependence. **A. Goel**, J. Luetzenkirchen, M.A. Brown

Section C
Ernest N. Morial Convention Center
Room 339

Impacts of Mining & Hydraulic Fracturing On Crop & Livestock Production
Cosponsored by AGFD, AGRO and ENVR
D. Alessi, T. Borch, N.R. Warner, *Organizers, Presiding*

1:30 GEOC 150. Pathways and mechanisms for natural attenuation of nonionic surfactants in hydraulic fracturing fluids if released to agricultural soil and groundwater. **P. Mouser**, K.M. Heyob, J. Blotevogel, J.J. Lenhart, T. Borch

2:00 GEOC 151. The response of soil microbial communities to hydraulic fracturing fluids. **S. Crowe**, N. Finke, J. Spence, R. Simister, A. Sturm

2:30 GEOC 152. Toxicological and chemical assessment of water quality downstream of NPDES oil and gas produced water discharges. **M. McLaughlin**, J. Blotevogel, B. McDevitt, N.R. Warner, R.L. Tanguay, E. Folkerts, T. Blewett, D. Alessi, G. Goss, J. Argueso, T. Borch

2:50 GEOC 153. Investigating enhanced sediment radium levels at NPDES facilities in Wyoming with a comparison to Pennsylvania. **B. McDevitt**, M. McLaughlin, J. Blotevogel, T. Borch, N.R. Warner

3:10 Intermission.

3:30 GEOC 154. Fate of organic additives in hydraulic fracturing fluids from injection through production and treatment. B. McAdams, K. Carter, J. Blotevogel, T. Borch, **J. Hakala**

3:50 GEOC 155. Elemental contaminants in produced water and their impact on treatment and reuse. **E.F. Peltier**, M. Chen, S. Randtke, K. Shafer-Peltier, M. Veisi, O. Dollar

4:10 GEOC 156. Oil and gas wastewater spreading on roads and associated environmental and human health impacts. **T. Tasker**, P. Piotrowski, L. Castillo, T. Blewett, K. Ganow, P. Delompre, J. Vanden Heuvel, F.L. Dorman, N.R. Warner, W.D. Burgos

4:30 GEOC 157. Risks for reuse of unconventional oil and gas wastewater. **A. Vengosh**, A.J. Kondash

Carbon Dioxide Conversion & Artificial Photosynthesis

Electro-Photo Catalytical Conversion

Sponsored by ENFL, Cosponsored by CATL, COMP and GEOC

Redox & Interfacial Dynamics Among Coupled Biogeochemical Cycles of Fe, S, Minerals & Organic Matter: Implications to Multiscale Behaviors of Contaminants, Carbon & Nutrients
Sponsored by ENVR, Cosponsored by GEOC

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 355

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Cosponsored by ENVR
W.D. Burgos, M.A. Ginder-Vogel, M. Zhu, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 158. Formation and reactivity of manganese oxides in the environment: field and laboratory results. **G.W. Luther**, V.E. Oldham, A. Thibault de Chanvalon, E.R. Estes, B.M. Tebo, M. Wright, M. Jones, M. Siebecker, A. Madison, A. Mucci

9:05 GEOC 159. The role of trivalent manganese in mineralogy and geochemistry of birnessite. **M. Zhu**

9:25 GEOC 160. Evolution of vernadite crystal structure as a function of pH: Implications for reactivity. S. Grangeon, **B. Lanson**

9:45 GEOC 161. Rapid transformation of layered to tunneled manganese oxide triggered by interlayer Mn(III). **P. Yang**, S. Lee, J. Post, H. Xu, Q. Wang, W. Xu, M. Zhu

10:05 Intermission.

10:30 GEOC 162. Structures and behaviors of birnessites. **J. Post**, P. Heaney, F.T. Ling

11:00 GEOC 163. Tracking the recrystallization and transformation of birnessite in reducing environments with ^{54}Mn radiotracers. **E. Elzinga**

11:30 GEOC 164. Manganese(IV) oxide formation by a bacterial manganese oxidase. **A. Soldatova**, C. Romano, L. Tao, T.A. Stich, W.H. Casey, R. Britt, B.M. Tebo, T.G. Spiro

12:00 GEOC 165. Understanding the redox reactivity of mycogenic manganese oxides. B. Uster, **J.A. Henson**, G.S. McCarty, J. Pena, L.A. Sombers, **O. Duckworth**

Section B
Ernest N. Morial Convention Center
Room 338

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Confinement: Clay Mineral Geochemistry

Cosponsored by ENVR and INOR
J. Bracco, S.E. Mason, J. Weber, *Organizers, Presiding*

8:30 GEOC 166. Optical imaging of surface chemistry and dynamics in confinement. C. Macias-Romero, I. Nahalka, H. Okur, **S. Roke**

8:50 GEOC 167. The interfacial structure of water droplets in a hydrophobic liquid. N. Smolentsev, W. Smit, H. Bakker, **S. Roke**

9:10 GEOC 168. The impact of nano-scale confinement on the adsorption of copper. **A. Knight**, A. Tigges, A. Ilgen

9:30 GEOC 169. Atomistic-scale evaluation of the fracture toughness of silicates in aqueous solutions. **J.M. Rimsza**, R.E. Jones, L.J. Criscenti

9:50 Intermission .

10:10 GEOC 170. Hydration structure of mineral–water interfaces. **S. Lee**, J. Bracco, I.C. Bourg, A.G. Stack, P. Fenter

10:40 GEOC 171. Free energy of interaction of two smectite clay nanoparticles in liquid water. **X. Shen**, I.C. Bourg

‡*Cooperative Cosponsorship*

11:00 GEOC 172. Metadynamics based molecular dynamics simulation and experimental study of the adsorption of phthalate esters on smectite clay surfaces. **J. Willemsen**, S.C. Myneni, I.C. Bourg

11:20 GEOC 173. Imaging nucleation at the mica-water interface with high speed molecular-resolution atomic force microscopy. **B. Legg**, M.D. Baer, C.J. Mundy, J.J. DeYoreo

11:40 GEOC 174. Properties of clay-rich fine-grained sedimentary rocks from large-scale molecular dynamics simulations. **T.R. Underwood**, I.C. Bourg

12:00 GEOC 175. Sugar-influenced hydrodynamics in mineral nanopores revealed by molecular dynamics simulations coupled with spectroscopic experiments. **L. Aristilde**, S. Kelch, S. Galdi

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 355

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Cosponsored by ENVR
W.D. Burgos, M.A. Ginder-Vogel, M. Zhu, *Organizers, Presiding*

1:30 GEOC 176. Transformation of phenolic contaminants by environmentally-relevant manganese oxides. **C.K. Remucal**, E. Leverich, M.A. Ginder-Vogel

2:00 GEOC 177. Biogenic manganese oxides from AMD treatment system remove contaminants of emerging concern from hospital wastewater. **L.E. Castillo**, P. Piotrowski, F.L. Dorman, J. Vanden Heuvel, W.D. Burgos

2:25 GEOC 178. Changes in bisphenol A oxidation mechanism in the presence of manganese oxide. **S.J. Balgooyen**, G. Campagnola, C.K. Remucal, M.A. Ginder-Vogel

2:45 GEOC 179. Application of different manganese dioxide (MnO_x) media for the removal of bisphenol A (BPA). **M.M. Shaikh**, H.J. Zhang, J.M. Cerrato

3:05 Intermission.

3:30 GEOC 180. Reduction of layered manganese oxides by organic acids: Effects on mineral structure and trace metal fate. **J.G. Catalano**, E.D. Flynn, M.A. Hinkle

4:00 GEOC 181. Reductive dissolution kinetics of birnessite by natural organic matter. **Q. Wang**, M. Zhu

4:20 GEOC 182. Decoupling flavin and thiol mediated reduction of manganese oxides by *Shewanella oneidensis* MR-1. **K. Michelson**, R. Sanford, A. Valocchi, C.J. Werth

4:40 GEOC 183. Reduction of manganese (oxyhydr)oxides by organic sulfur electron shuttles. **E. Eitel**, S. Zhao, Y. Tang, M. Taillefert

Section B
Ernest N. Morial Convention Center
Room 338

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Carbonates, Phosphates & Rare Earth Elements

Cosponsored by ENVR and INOR
J. Bracco, S.E. Mason, J. Weber, *Organizers, Presiding*

1:30 GEOC 184. Molecular scale structure of the calcite(104)-water-interface and interfacial reactions of Selenite ($Se(IV)O_3^{2-}$), insights from experiment and theory. **F. Heberling**, R. Polly

2:00 GEOC 185. *Ab initio* thermodynamics of hydrated Mg and Ca carbonates. **A.M. Chaka**

2:30 GEOC 186. Molecular scale mechanisms of heteroepitaxial nucleation and growth at mineral-water interfaces. **S.L. Riechers**, M. Xu, E.S. Ilton, Y. Du, L. Kovarik, T. Varga, B. Arey, O. Qafoku, K. Rosso, S.N. Kerisit

3:00 GEOC 187. $CaCO_3$ heterogeneous nucleation pathways: Effect of mineral surface hydrophobicity. **A. Koishi**, A. Fernandez-Martinez, A. van Driessche, L. Michot, G. Montes-Hernandez, B. Lee

3:20 Intermission .

3:40 GEOC 188. Linking computational simulation with neutron diffraction to understand ion solvation structure and ion pairing in aqueous solutions. **A.G. Stack**, H. Wang, J. Neuefeind, N. Rampal, J.M. Simonson

4:10 GEOC 189. ATR-FTIR analysis of ligand adsorption at the mineral-solution interface. **A.K. Wanhala**, A.G. Stack, M. Cheshire, V.S. Bryantsev

4:30 GEOC 190. Influence of organic ligands on the mobilization and pattern of rare earth elements. **P. Liu**, Y. Tang

4:50 GEOC 191. Divalent metal sorption on struvite: Assessing the influence of pH and concentration on sorption mechanisms. **O. Goswami**, A. Rouff

Section C
Ernest N. Morial Convention Center
Room 339

Forensic Geochemistry
Cosponsored by ENVR
D. Coleman, S. Singletary, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 GEOC 192. Forensic geology. **R. Murray**

2:05 GEOC 193. Forensic use of the electron microprobe. **S. Singletary**, H. Hanna

2:20 GEOC 194. Forensic chemical and geochemical evaluation of seepage fluids and groundwater in a semi-controlled dumping site in northern Croatia. **G. Kniewald**, M. Mlakar

2:35 Intermission.

2:55 GEOC 195. Nuclear forensic analysis of uranium dioxide fuel pellets. **T.L. Spano**, L. Corcoran, A. Simonetti, C. Dorais, S. Lewis, T. Gunther, P.C. Burns

3:10 GEOC 196. Chromium in aqueous media: How to determine source and speciation with limited data. **K. Thorbjornsen**

3:25 GEOC 197. Monitoring on styrene oligomer derived from debris polystyrene world wide. **K. Saido**, H. Kimukai, B. Brezel, **K. Koizumi**, D.M. Karl, N. Maximenko, B. Kwon, S. Chung, M. Ochiai

3:40 Concluding Remarks.

WEDNESDAY EVENING

Section C
Ernest N. Morial Convention Center
Hall D

Biomineralization & Bio-Compatible Minerals
Cosponsored by BIOL and ENVR
J.D. Rimer, J.A. Soltis, G. Zhu, *Organizers*

6:00–8:00

GEOC 198. MapX – An *in situ*, full-frame X-ray spectroscopic imager for planetary science and astrobiology. **R.C. Walroth**, P. Sarrazin, T. Bristow, D. Blake

GEOC 199. *In-situ* morphological and structural transformation of abiogenic and biogenic iron-sulfide nanoparticles: An X-ray scattering and transmission electron microscopy study. **E.A. Moreno Flores**, J. Banuelos, J. Xu

Section C
Ernest N. Morial Convention Center
Hall D

Contaminated Site Remediation through Microbial, Geological & Chemical Processes
Cosponsored by ENVR
B. Jeon, Y. Ok, D. Tsang, *Organizers*

6:00–8:00

GEOC 200. EXAFS and μXRF analysis of arsenic speciation and spatial distribution in mine tailings: Implications for physical weathering, bioaccessibility, and remediation. **M.R. Vejar**, C.J. Reilly, C.S. Kim

GEOC 201. Microspatial analysis of arsenic oxidation state in mine tailings: Implications for bioaccessibility and remediation. **C.J. Reilly**, M.R. Vejar, C.S. Kim

GEOC 202. Degradation in low-temperature thermal remediation: Mechanisms and mineral catalysis. **J. Davis**, C. Oden, H. Liljestrand, C.J. Werth, L.E. Katz

GEOC 203. Degradation of TCE by iron minerals and aquifer materials. **T.C. Robinson**, M. Scherer, D. Latta, T. Mattes, P. Richards, A. Neumann, J. Entwistle, E. Suchomel, R. Deeb, L. Kane

GEOC 204. Pyrolytic treatment for the remediation of crude oil contaminated soil. **J. Jang**, S. Dev, S. Lee, B. Jeon

GEOC 205. Sediment core depth profile enhanced degradation of CFCs by biotic and abiotic in-situ stimulation. **N. Gambrell**, **C. Masse**, S.K. O'Shea

GEOC 206. Characterization of in-situ marine core sediment and pore water degradation of CFCs. **C. Masse**, N. Gambrell, S.K. O'Shea

GEOC 207. Reduction of Hg(II) by structural Fe(II) in clay minerals. K.O. Thalhammer, M. Boyanov, K.M. Kemner, **E.J. O'Loughlin**

GEOC 208. Wood biochar as cattle feed supplement: Effect on milk yield and nutrient quality in the farms of West Bengal, India. **J. Bhattacharya**, B. Das

Section C
Ernest N. Morial Convention Center
Hall D

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Cosponsored by COLL, ENFL, ENVR and INOR
N. Kabengi, M.L. Machesky, A. Navrotsky, *Organizers*

6:00–8:00

GEOC 209. Fluid behaviors in natural confinement systems. **B. Hwang**, D.J. Srivastava, T. Whitmer, S. Ok, A. Swift, P.J. Grandinetti, D. Cole

GEOC 210. Thermodynamic analysis of alkali metal ions (Li^+, Na^+, K^{+}) exchange on MXene using flow microcalorimetry. **E. Stroeva**, P. Ilani Kashkouli, M. Naguib, D. Wesolowski, N. Kabengi

GEOC 211. Withdrawn.

Section C

Ernest N. Morial Convention Center
Hall D

Forensic Geochemistry
Cosponsored by ENVR
D. Coleman, S. Singletary, *Organizers*

6:00–8:00

GEOC 212. Geochemical fingerprinting of uranium rich samples utilizing a multivariant approach. **L. Corcoran**, T.L. Spano, A. Simonetti, S. Lewis, T. Gunther, P.C. Burns

GEOC 213. Calcium and iron isotope analysis of uraninite and other uranium-rich materials: Development of potential new forensic isotope tracer methods. **T. Gunther**, L. Corcoran, A. Simonetti, P.C. Burns

GEOC 214. Detailed in-situ characterization of uraninite from North American deposits using a combined FIB-SEM approach. **S. Lewis**, A. Simonetti, L. Corcoran, T.L. Spano, P.C. Burns

Section C
Ernest N. Morial Convention Center
Hall D

General Geochemistry

W.D. Burgos, N. Kabengi, *Organizers*

6:00–8:00

GEOC 215. Investigation of the reactions of NO_x species with pyrite(FeS_2). **T. Rush**, H. Bevsek

GEOC 216. Laboratory study of interfacial processes of herbicides. **P. Orlović-Leko**, K. Vidović, I. Ciglenečki

GEOC 217. The study of interaction of bacterial cytochromes and iron oxide minerals. **H. Wang**, A. Johs, L. Liang, J. Browning, A. Tennant

GEOC 218. Oxidized manganese in Costa Rican tree leaves. **R.L. Sanders**, J. Sager, A. Schwarz

GEOC 219. Study of iodine distribution in western Oklahoma brine waters. **J.R.**

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Wickham, K. Betz, M. Archer, D. Edlin

GEOC 220. NMR correlation spectroscopy of liquids at geochemical pressures (GPa). **G. Ochoa**, J.D. Kerr, W.H. Casey, M.P. Augustine

GEOC 221. Resolving the spatial distribution of siderophores and other metabolites at lichen-mineral interface. **B.P. Fields**, J. Thieme, K. Haselwandter, Y. Tang

GEOC 222. Bioreduction of iron in pyroaurite by *Shewanella putrefaciens* CN32. M. Ramos, M. Boyanov, K.M. Kemner, **E.J. O'Loughlin**

GEOC 223. Development of a new method for CEC determination of clays. A.S. Frantzen, **C.A. Keith**

GEOC 224. Methylmercury levels in cover soils from two landfills in Xi'an and Shanghai, China: Evidence for inactive sites of methylmercury production. **Z. Tao**

Section C
Ernest N. Morial Convention Center
Hall D

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Cosponsored by ENVR
W.D. Burgos, M.A. Ginder-Vogel, M. Zhu, *Organizers*

6:00–8:00

GEOC 225. Effects of cations on structural transformation of birnessite by fulvic acid under anoxic conditions. **Q. Wang**, P. Yang, M. Zhu

GEOC 226. Effects of ligands on structural transformation of birnessite during the reaction with Mn(II). **P. Yang**, Q. Wang, M. Zhu

Section C
Ernest N. Morial Convention Center
Hall D

Microbially-Driven Geochemical Reactions: Kinetics & Communities
Cosponsored by BIOL and ENVR
W.D. Burgos, C. Chan, S. Crowe, *Organizers*

6:00–8:00

GEOC 227. Mapping the potential for functional redundancy in iron-oxidizing communities using pathway-centric analysis. **D. Ayala**, R. Simister, S. Crowe, S. Hallam, W.D. Burgos

Section C
Ernest N. Morial Convention Center
Hall D

Mineral-Water Interface Geochemistry & Modeling at the Laboratory- & Field-Scales: Symposium in Honor of James A Davis
Cosponsored by ENVR
K. Campbell, M.B. Hay, D.B. Kent, *Organizers*

6:00–8:00

GEOC 228. Passivation of uranium ore material surfaces with uranyl phosphate precipitation. **T. Kane**, K. Campbell, M.B. Hay

GEOC 229. Chemical forms of sediment-bound Fe(II) in sediments from an aquifer contaminated by a petroleum spill. **M. Kohler**, D.B. Kent, I.M. Cozzarelli, E. Elzinga, K. Scheiderich, B.A. Bekins

GEOC 230. Surface complexation and reactive transport modeling: An environmental consultant's perspective. **M.B. Hay**, P. Moran, J. Gillow

Section C
Ernest N. Morial Convention Center
Hall D

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments
Cosponsored by ENVR and INOR
J. Bracco, S.E. Mason, J. Weber, *Organizers*

6:00–8:00

GEOC 231. Modelling of solid-liquid interactions using scaled charges in accord with the Electronic continuum correction. D. Biriukov, **M. Predota**, O. Kroutil, Z. Chval, M. Kabelac

GEOC 232. Sorption of pyridine cations to aluminosilicate clays: Influence of solid phase composition and structure. **S. Shaheen**, D. Freeman, J. Sullivan, D. Vasudevan

GEOC 233. Photochemical cycling of reactive cxygen cpecies in hydrothermal springs: Impacts on biosignature preservation. **M. Mave**, N. Hinman

Section C
Ernest N. Morial Convention Center
Hall D

Multiscale Biogeochemical Processes in Soil Ecosystems: Critical Reactions & Resilience to Climate Changes
Cosponsored by AGRO and ENVR
M. Keiluweit, B. Xing, Y. Yang, *Organizers*

6:00–8:00

GEOC 234. Assessing environmentally persistent free radical formation potential and redox processes in Louisiana wetland soils undergoing erosion. **E. Ampiah**, B.J. Haywood, J.R. White, R.L. Cook

GEOC 235. Time-lapse view of carbon fluctuations in of the Mississippi River. **M.P. Hayes**, B.J. Haywood, F. Scaglia Drusini, R.L. Cook

GEOC 236. Integrating laboratory and field studies of organo-mineral interactions using multiple spectroscopic methods. **W. Atkinson**, R. Sleighter, T. Regier, P.G. Hatcher, S.C. Myneni

Section C
Ernest N. Morial Convention Center
Hall D

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Cosponsored by ENVR and INOR
G.M. Bowers, R. Kirkpatrick, N. Loganathan, *Organizers*

6:00–8:00

GEOC 237. Grand canonical molecular dynamics simulation of supercritical carbon dioxide and methane intercalation in smectite interlayers. **N. Loganathan**, O. Yazaydin, G.M. Bowers, A.G. Kalinichev, R. Kirkpatrick

GEOC 238. Understanding alternative shale gas extraction technologies: Comparing and contrasting supercritical methane and carbon dioxide interactions with smectite clay on the molecular scale using *in situ* spectroscopy and diffraction. **G.M. Bowers**, S. Cunniff, H.T. Schaef, J. Loring, S. Burton, E.D. Walter, D.W. Hoyt, O. Yazaydin, N. Loganathan, R. Kirkpatrick

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 355

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Cosponsored by ENVR
W.D. Burgos, M.A. Ginder-Vogel, M. Zhu, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 GEOC 239. Redox reactivity of layer-type MnOx nanoparticles: Insights from kinetic and site-specific surface speciation studies. **J. Pena**, A. Simanova, Y. Wang, F. Marafatto, S. Benkaddour

9:05 GEOC 240. Cation exchange and redox reactions in birnessite as revealed by time-resolved X-ray diffraction. **P. Heaney**, J. Post, F.T. Ling, K. Kong, C.L. Lopano, C.R. Parasida, J. Stubbs, P.J. Eng

9:35 GEOC 241. Cr(VI) generation from Cr(III)-containing iron oxides associated with manganese redox cycling. **C. Pan**, A. Qian, J.G. Catalano, D. Giammar

9:55 GEOC 242. Shining light on Cr(III) oxidation mechanisms on Mn-oxides. **J. Fischel**, D.L. Sparks

10:15 Intermission.

10:40 GEOC 243. Efficient catalytic As(III) oxidation on the surface of ferrihydrite in the presence of aqueous Mn(II). **X. Feng**, S. Lan, H. Ying, X. Wang, F. Liu, W. Tan, Q. Huang

11:10 GEOC 244. Reactivity of manganese oxide at redox interfaces in diffusion controlled environments. **S. Ying**, M. Abernathy, R. Mock, J. Lezama, A. Garniwan, L. Lake, I. Lee, M.V. Schaefer

11:40 GEOC 245. Arsenic oxidation by the mighty manganese soils of Graskop. **M. Fischel**, C. Clarke, D.L. Sparks

12:00 GEOC 246. Impact of metal impurities on redox reactivity of hausmannite ($Mn^{II}Mn^{III}_2O_4$). **B. Song**, E.B. Cerkez, D.R. Strongin, B. Kim

Section B
Ernest N. Morial Convention Center
Room 338

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Iron Oxyhydr-Oxides: Redox Processes

Cosponsored by ENVR and INOR
J. Bracco, S.E. Mason, J. Weber, *Organizers, Presiding*

8:30 GEOC 247. Ions and solvent structure at mineral- aqueous interfaces. **E. Borguet**

9:00 GEOC 248. Carbonate adsorption on ferrihydrite under atmospheric conditions: Experimental and modeling. **N.M. Bompoti**, M. Chrysochoou, M. Villalobos, M.L. Machesky

9:20 GEOC 249. Quantifying rates and extents of Fe^{2+} catalyzed iron oxide recrystallization. **P. Joshi**, M.S. Fantle, C. Gorski

9:40 GEOC 250. Adsorption of nucleic acid/protein supramolecular complexes on goethite: Impact of solution interactions on behavior at the solution-mineral interface. **M. Schmidt**, C.E. Martinez

10:00 GEOC 251. Reconstituting the Fe L-edge and O K-edge XANES and XMCD spectra of magnetite from first principle calculations. **M. Sassi**, C. Pearce, P.S. Bagus, E. Arenholz, K. Rosso

10:20 Intermission.

10:30 GEOC 252. X-ray absorption, Mössbauer, diffuse reflectance spectroscopies and density functional theory calculations of Fe(II)/Fe(III) redox couple in ferric nontronites. **A. Ilgen**, R. Kukkadapu, R.E. Washington, K. Leung

10:50 GEOC 253. Mediated electrochemical reduction of iron (oxyhydr-)oxides under defined thermodynamic boundary conditions. M. Aeppli, A. Voegelin, C. Gorski, **T.B. Hofstetter**, M. Sander

11:10 GEOC 254. Unifying framework to relate pollutant reduction rates by oxide-bound Fe(II) to thermodynamics. S. Stewart, T.B. Hofstetter, P. Joshi, **C. Gorski**

11:30 GEOC 255. Role of defects in Fe(II)–goethite electron transfer. **L. Andrade**, D. Latta, A. Neumann, C. Pearce, M. Sassi, A. N'Diaye, K. Rosso, M. Scherer

11:50 GEOC 256. Redox degradation of DTPMP phosphonate with Fe-bearing phyllosilicates under subsurface conditions. **L. Zhang**, Y. Jun

12:10 GEOC 257. Confinement-induced solvent effects on electron transfer reactions at water-mineral interfaces. **R. Remsing**

Section C
Ernest N. Morial Convention Center
Room 339

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Cosponsored by ENVR and INOR
G.M. Bowers, R. Kirkpatrick, N. Loganathan, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 GEOC 258. Properties of water under ultra-confinement: Questions about the subsurface. **L. Anovitz**, A.I. Kolesnikov, C. Hoffmann, G. Reiter, T. Prisk, P. Kent, E. Mamontov, D. Wesolowski

9:10 GEOC 259. Molecular dynamics simulation prediction of quartz wetting by water vs. supercritical CO_2. E. Sun, E. Chang, L.N. Lammers, **I.C. Bourg**

9:40 GEOC 260. Impact of small organic molecules on the wettability of quartz by brine versus CO_2. **E. Sun**, I.C. Bourg

10:00 GEOC 261. Reactivity and transformations of minerals in adsorbed H_2O films. **J. Loring**, Q. Miller, H.T. Schaef, E. Ilton, O. Qafoku, C.J. Thompson, P. McGrail, K. Rosso

10:30 Intermission.

10:40 GEOC 262. Interactions of water

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and supercritical carbon dioxide on the basal surface and interlayer of clay minerals. **R.T. Cygan**

11:10 GEOC 263. Getting the lead out: The unusual carbonation chemistry of a Pb-smectite in contact with wet supercritical carbon dioxide. **G.M. Bowers**, S. Cunniff, H.T. Schaef, S. Burton, J. Loring

11:30 GEOC 264. Investigation of geochemically relevant supercritical fluids interaction with clay minerals present in deep geological formations using grand canonical molecular dynamics (GCMD). **N. Loganathan**, O. Yazaydin, G.M. Bowers, A.G. Kalinichev, R. Kirkpatrick

11:50 GEOC 265. Gas and supercritical fluid adsorption at mineral surfaces, in narrow pores, and to swelling clays: Impacts of hydration and fluid identity. **G. Rother**, D. Cole, I.C. Bourg, M. Cheshire, L. Vlcek

12:20 Concluding Remarks.

THURSDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 355

Manganese Oxides: Their Formation, Structure, Reactivity & Applications
Cosponsored by ENVR
W.D. Burgos, M.A. Ginder-Vogel, M. Zhu, *Organizers, Presiding*

1:30 GEOC 266. Thallium (I) sorption behavior on birnessite. **M. Villalobos**, Y. Cruz-Hernandez, M.A. Marcus

2:00 GEOC 267. Adsorption behavior of Mn(II) on the surface of Fe (oxyhydr) oxides under various aqueous conditions. **S. Namgung**, G. Lee

2:20 GEOC 268. Potential role of Mn(IV) oxides in abiotic nitrous oxide production. **A. Cavazos**, M. Taillefert, Y. Tang, J. Glass

2:40 Intermission.

3:00 GEOC 269. Electrochemical characterization of manganese oxide electrodes for water desalination and renewable energy production. **C. Gorski**, J. Fortunato, T. Kim, B.E. Logan

3:30 GEOC 270. Withdrawn.

3:50 GEOC 271. Previously unexplored fast photochemical oxidation of Mn^{2+} (aq) in an abiotic inorganic process and consequent formation of birnessite nanosheets. H. Jung, **Y. Jun**

Section B
Ernest N. Morial Convention Center
Room 338

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Uranium Incorporation: Sulfate Mineral Geochemistry

Cosponsored by ENVR and INOR
J. Bracco, S.E. Mason, J. Weber, *Organizers, Presiding*

1:30 GEOC 272. Illuminating uranium incorporation in iron (oxyhydr)oxides using AIMD-informed EXAFS analysis. **M.E. McBriarty**, S.N. Kerisit, E.J. Bylaska, J.A. Soltis, S. Shaw, E. Ilton

1:50 GEOC 273. Evolution of uranium speciation during sulfidation of iron (oxyhydr)oxides under conditions relevant to geological disposal of radioactive waste. **L.T. Townsend**, S. Shaw, J.W. Mosselmans, A. Walton, R. Hibberd, K. Morris

2:10 GEOC 274. Uranium(VI) uptake during iron(III) (oxyhydr)oxide formation: Underpinning radioactive effluent treatment. **E. Winstanley**, K. Morris, L. Abrahamsen-Mills, S. Haigh, S. Shaw

2:30 GEOC 275. Stability and core-shell structure of U(IV)-silicate colloids. **T. Neill**, K. Morris, C. Pearce, N.K. Sherriff, S. Shaw

2:50 Intermission .

3:10 GEOC 276. Withdrawn.

3:30 GEOC 277. Designing inhibitors of mineral scale: A new platform based on cooperative microfluidic and computational assays. **R. Sosa**, X. Geng, J. Palmer, M.A. Reynolds, J. Conrad, J.D. Rimer

3:50 GEOC 278. Heterogeneous $(Ba_xSr_{1-x})SO_4$ nucleation at organic-water interfaces: Implications for strontium immobilization. **N. Deng**, B. Cao, X. Zuo, Y. Hu

4:10 GEOC 279. Strontium adsorption at the barite (001) – water interface. **J. Bracco**, S. Lee, J. Stubbs, P.J. Eng, J. Weber, P. Fenter, J.D. Kubicki

Section C
Ernest N. Morial Convention Center
Room 339

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Cosponsored by ENVR and INOR
G.M. Bowers, R. Kirkpatrick, N. Loganathan, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 GEOC 280. Behavior of supercritical C-O-H fluids in nanoporous materials. **D. Cole**, A. Striolo, S. Gautam

2:05 GEOC 281. Molecular simulations of competitive sorption of carbon dioxide and methane on illitic clay surfaces in shales. **E.M. Myshakin**, L. Chong, D. Crandall

2:35 Intermission.

2:45 GEOC 282. Geochemical and geomechanical alteration of reservoir rock by CO_2-saturated brine following carbon sequestration. **S. Fuchs**, L.A. Hernandez, A. Akono, D.N. Espinoza, C.J. Werth

3:05 GEOC 283. Cavity formation in aqueous solutions and molecular origin of salting-out effect for CO_2. **T.A. Ho**, A. Ilgen

3:25 Discussion.

5:25 Concluding Remarks.

HIST

Division of the History of Chemistry

N. Tsarevsky, *Program Chair*

SUNDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 24

Tutorial & General Papers

N.V. Tsarevsky, *Organizer*
J.S. Jeffers, *Presiding*

8:00 HIST 1. Chemistry in America: Seventeenth century New England and John Winthrop, Jr.. **G.D. Patterson**

8:30 HIST 2. Withdrawn.

9:00 HIST 3. Early German influences on women in chemistry. **R.C. White**

9:30 HIST 4. Solving crime mysteries using chemistry: The early days of forensic science. **N.V. Tsarevsky**

10:00 Intermission.

10:15 HIST 5. Bibliometric overview of drug repurposing using PubMed. **N. Baker**, A.J. Williams, S. Ekins, A. Tropsha

10:45 HIST 6. History of Ethyl Corporation in Baton Rouge, Louisiana and beyond. **C.D. Varnado**

11:15 HIST 7. History of cyclic polymers. **F.M. Haque**, S.M. Grayson

11:45 HIST 8. John Herschel as a chemist. **G.D. Patterson**

SUNDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 24

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡
Financially supported by ACS Louisiana Local Section
A.F. Bopp, *Organizer*
M. Orna, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 HIST 9. Impact of agriculture on food supply: A history. **L. Simon Sarkadi**

1:40 HIST 10. Critical impact of NaCl on global human history and development. **M. Duerst**

2:10 HIST 11. Sweet chemistry: A philatelic history of sugar. **D. Rabinovich**

2:40 Intermission.

3:00 HIST 12. History of sugar and sweeteners. **G. Eggleston**

3:30 HIST 13. Uncorking the past: Alcoholic beverages as the universal medicine before synthetics. **P.E. McGovern**

4:00 HIST 14. Why we do this to ourselves? The chemical/botanical history of chili peppers. **R. Mullin**

4:30 Concluding Remarks.

MONDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 24

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡
Financially supported by ACS Louisiana Local Section
A.F. Bopp, M. Orna, *Organizers*
D. Rabinovich, *Presiding*

8:30 Introductory Remarks.

8:40 HIST 15. Cuisine and chemistry: From Liebig's "Dietetic Trinity" to molecular gastronomy. **L. Civitello**

9:10 HIST 16. Harvey Wiley and the transformation of the American diet. **J. Rees**

9:40 HIST 17. History of dietary guidelines and their impacts. **E. Schoffers**

10:10 Intermission.

10:30 HIST 18. Eating chemicals: The flavor industry and its chemical relations. **N. Berenstein**

11:00 HIST 19. Genetically modified organisms (GMOs) as part of our food sources: Are you what you eat? **P.L. Daubenmire**

11:30 HIST 20. Carotenoids, cochineal and copper: Food coloring through the ages. **M. Orna**

12:00 Concluding Remarks.

Molecules that Changed the World
Sponsored by YCC, Cosponsored by HIST and I&EC

MONDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 24

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡
Financially supported by ACS Louisiana Local Section
M. Orna, *Organizer*
A.F. Bopp, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 HIST 21. How food culture survives and thrives in a changing world. **P. Tooker**

2:40 HIST 22. Evolution of flour: From New England Graham to New Orleans Swans Down. **L. Civitello**

3:10 Intermission.

3:30 HIST 23. Effects of fertilizer on food supply. **L. Simon Sarkadi**

4:00 HIST 24. Role of chemical analysis in food safety and food authentication. **E. de Ronde**

4:30 HIST 25. What 18 inches could mean? Relative sea level rise and Louisiana. **A. Gaudé**

5:00 HIST 26. Student/teacher essay contest winners: The best in the chemical history of food. S.C. Rukes, **M. Orna**

5:30 Concluding Remarks.

‡*Cooperative Cosponsorship*

Information Legacy of Eugene Garfield: From the Chicken Coop to the World Wide Web
Sponsored by CINF, Cosponsored by HIST and PRES

Tales of Chemistry & Cocktails
Sponsored by YCC, Cosponsored by HIST

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
N.V. Tsarevsky, *Organizer*

8:00–10:00

7. See previous listings.

31, **45**, **48**-**49**. See subsequent listings.

TUESDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 24

HIST Award Symposium Honoring Jeffrey I. Seeman

J. Gal, *Organizer, Presiding*

8:25 Introductory Remarks.

8:30 HIST 27. Seeman, Padwa, Gupton and five membered heterocycles: How organic chemistry brought us together. **J.T. Gupton**

9:00 HIST 28. Two examples of serendipity in my scientific career. **E. Juaristi**

9:30 HIST 29. My journey from a never-heard land to ... to the land of opportunities. **M. Hajaligol**

10:00 HIST 30. Thoughts on the relevance of history. **M. Caserio**

10:30 Intermission.

10:45 HIST 31. Publishing chemical history: Lessons learned. **E.E. Wille**

11:15 HIST 32. Resilience: When life hands you a lemon, make lemonade. **M. Rouhi**

11:45 HIST 33. History of and history in *Angewandte Chemie*. **P.K. Goelitz**

TUESDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 24

HIST Award Symposium Honoring Jeffrey I. Seeman

J. Gal, *Organizer, Presiding*
M. Orna, J. Seeman, *Presiding*

1:00 HIST 34. Reflections on the relationships of error to discovery in chemistry. **C.J. Giunta**

1:30 HIST 35. Origins: God or no God, that is the question. **M.T. Bowers**

2:00 HIST 36. Chemical receptors and transduction events on the mammalian tongue. **S. Simon**

2:30 HIST 37. Three evocative ideas: The Matthew effect, post mature contributions and the role of the role model. **H. Zuckerman**

3:00 Intermission.

3:15 HIST 38. Best of all possible worlds. **R. Anderson**

3:45 HIST 39. "Go for it": Words of wisdom from my fathers. **L.M. Shea**

4:15 HIST 40. FDA history, drug inspection and compliance overview. **B. Higgins**

4:45 HIST 41. Emergence of molecular reaction dynamics. **D.R. Herschbach**

WEDNESDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 24

Tutorial & General Papers

N.V. Tsarevsky, *Organizer, Presiding*

8:15 HIST 42. History of the American chemical laboratory manual. **W.P. Palmer**

8:45 HIST 43. Victor Grignard (1871-1935) and Henry Gilman (1893-1986): Pioneers in organometallic chemistry. **R.K. Dieringer**, **H.K. North**, D.E. Lewis

9:15 HIST 44. Wolff-Kishner reduction: Biography, discovery and development. **D.E. Lewis**

9:45 HIST 45. Development of Butlerov's Structural Theory, 1859-1862. **C.S. Goedhart**, **D.R. Rothbauer**, S.N. Raspel, D.E. Lewis

10:15 Intermission.

10:30 HIST 46. Mining of elements versus discovery, analysis, and separation of elements. **C. Hahn**

11:00 HIST 47. August Michaelis: A pioneer of phosphorus chemistry. **D. Selent**

11:30 HIST 48. Markovnikov on isomerism in organic chemistry. **D.E. Lewis**

12:00 HIST 49. Mutual influence of atoms in chemical compounds—Markovnikov's Rule. **D.E. Lewis**

I&EC

Division of Industrial and Engineering Chemistry

C. Abney, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards:

Symposium in Honor of Ning Yan (see *CELL*, Sun)

Polymer Colloids: Synthesis, Analysis, Modeling & Applications (see *POLY*, Sun, Mon, Tue, Wed)

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Rafael Luque (see *CELL*, Mon)

Industrial Innovations in Polymer Science (see *POLY*, Mon)

BUSINESS MEETINGS:

I&EC Subdivision Meeting (Open), 10:00 AM: Sat

I&EC Business Meeting (Open), 1:00 PM: Sat

SUNDAY MORNING

Section A
Loews New Orleans Hotel
Louisiana I

E.V. Murphree Award in Industrial and Engineering Chemistry: Symposium in honor of Linda J. Broadbelt

Cosponsored by WCC
D.J. Klinke, H. Kung, *Organizers*
B.H. Shanks, *Presiding*

8:00 Introductory Remarks.

8:05 I&EC 57. Withdrawn

8:35 I&EC 1. Software tools for molecular-level modeling of refinery and petrochemical reactors. **M.T. Klein**

9:05 I&EC 3. Severe pyrolyses of n-decane, cyclodecane, and decahydronaphthalene, with graph-theoretic interpretations. **P.S. Virk**

9:35 Intermission.

9:55 I&EC 4. Application of molecular dynamics to discover and quantify reaction pathways. **J. Pfaendtner**, C. Fu

10:25 I&EC 5. Reaction mechanisms in industrial and engineering chemistry: from pyrolysis to proteins. **H. Mayes**

10:55 I&EC 6. From petrochemical reaction networks to intercellular networks in cancer: Developing ways to let reactive systems speak for themselves. **D.J. Klinke**

Section B
Loews New Orleans Hotel
Feliciana East

I&EC Fellow: Symposium in Honor of Yong Wang

J.L. Bryant, *Organizer*
J. Holladay, J. McEwen, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 7. Consequences of surface reconstruction of perovskites in catalyzing acid-base reactions. **Z. Wu**

8:30 I&EC 8. Structural and mechanistic insights from *in situ/operando* catalyst characterization. **A.M. Karim**

8:55 I&EC 9. Application of ambient pressure photoelectron spectroscopy to catalysis studies. **F. Tao**

9:20 I&EC 10. Direct conversion of syngas into lower olefins and aromatics with bifunctional catalysts. K. Cheng, W. Zhou, J. Kang, Q. Zhang, **Y. Wang**

9:45 Intermission.

10:05 I&EC 11. Enhancing the stability/performance of catalysts via atomic layer deposition. **C.L. Marshall**, H. Zhang, J. Camacho-Bunquin, J. Elam, R. Kennedy, P.C. Stair, K.R. Poeppelmeier

10:30 I&EC 12. Metal-incorporated silicates via evaporation-induced self-assembly as superior catalytic materials. A. Ramanathan, H. Zhu, J. Wu, S.K. Maiti, **B. Subramaniam**

10:55 I&EC 13. Cu/SSZ-13 catalysts for the selective catalytic reduction of NOx: Unusual features of the complex redox reaction mechanism. **C.H. Peden**, D. Mei, Y. Wang, J. Szanyi, F. Gao

11:20 I&EC 14. Catalysis researchers caused climate change and what we can do to fix it. **C.W. Jones**

Section C
Loews New Orleans Hotel
Louisiana II

ACS Award in Separations Science & Technology: Symposium in honor of Massimo Morbidelli

P. Arosio, M. Lattuada, A. Varma, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 15. Engineering an intein with cleavage control for single step purification platforms. **G. Belfort**

8:25 I&EC 16. Adapting process engineering to (bio)chemists for the development of smarter processes. **R.M. Nicoud**

8:45 I&EC 17. Continuous cell culture and purification processes for the integrated manufacture of monoclonal antibodies. **D.J. Karst**, F. Steinebach

9:05 I&EC 18. Simple approach to design chromatographic processes for mAb capture. **D.E. Pfister**, R.M. Nicoud

9:25 Intermission.

9:45 I&EC 19. Recent advances in understanding the molecular basis of selectivity in multimodal protein separation systems. **S.M. Cramer**

10:05 I&EC 20. Solution complexation: A methods to improve purity and yield in crystallization. **A.S. Myerson**

10:25 I&EC 21. Ligand-mediated nanocrystal growth. **S. Lazzari**, K.F. Jensen

10:45 I&EC 22. Enabling adsorbent screening for post-combustion CO2 capture through process optimization. **A. Rajendran**

11:05 I&EC 23. Award Address
(ACS Award in Separations Science and Technology Sponsored by the Waters Corporation). End-to-end integrated continuous manufacture of therapeutic proteins. **M. Morbidelli**

11:35 Concluding Remarks.

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

‡*Cooperative Cosponsorship*

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

SUNDAY AFTERNOON

Section A
Loews New Orleans Hotel
Louisiana I

E.V. Murphree Award in Industrial and Engineering Chemistry: Symposium in honor of Linda J. Broadbelt

Cosponsored by WCC
H. Kung, *Organizer*
D.J. Klinke, *Organizer, Presiding*

1:30 Introductory Remarks.
1:35 I&EC 24. Award Address (E.V. Murphree Award in Industrial and Engineering Chemistry Sponsored by the ExxonMobil Research and Engineering Company). Reaction pathway analysis of the (bio)conversion of (bio) macromolecules. **L.J. Broadbelt**

2:15 I&EC 25. Next generation chemical products via bioprivileged molecules. **B. Shanks**

2:45 I&EC 26. Computational framework for the identification of bioprivileged molecules. **X. Zhou**, Z. Brentzel, B.H. Shanks, J.A. Dumesic, L.J. Broadbelt

3:15 Intermission.

3:35 I&EC 27. Hybrid biological and catalytic processing to produce acrylonitrile. **G. Beckham**, E. Karp, T. Eaton, V. Sànchez i Nogué, V. Vorotnikov, M. Biddy, A. Bratis

4:05 I&EC 28. Kinetic analysis of phosphorylation of chimeric antigen receptors: Insight for T cell immunotherapy. **S. Finley**

4:35 I&EC 29. Interfacial perimeter sites for selective hydrocarbon oxidation over supported Au catalysts. **H. Kung**, M. Kung

Section B
Loews New Orleans Hotel
Feliciana East

I&EC Fellow: Symposium in Honor of Yong Wang

J.L. Bryant, *Organizer*
J. Holladay, J. McEwen, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 I&EC 30. Cascade catalysis: A strategy for process intensification. S. Eady, W. Wen, Z. Wang, **L.T. Thompson**

1:35 I&EC 31. Catalysis for C-C coupling and oxygen removal reactions of oxygenates at acid-base pairs on oxide surfaces. S. Wang, **E. Iglesia**

2:05 I&EC 32. Dynamics of first row transition metal or alloy clusters and their catalytic consequences for C-H bond dissociation and formation steps. **Y. Chin**, P.T. Lachkov, W. Tu

2:35 I&EC 33. Electrocatalytically-assisted oxidative dehydrogenation (ODH) of ethane. **U.S. Ozkan**, D. Dogu, K. Meyer, S. Gunduz, D.J. Deka, A. Co

3:05 Intermission.

3:20 I&EC 34. Structure-activity relationships for catalytic and photocatalytic reactions on nanocrystalline metal oxides: Bridging the materials gap. P. Pepin, **J.M. Vohs**

3:50 I&EC 35. On the various mechanisms of hydrodeoxygenation and ring hydrogenation of phenolics on metals. **D.E. Resasco**, N. Duong, Q. Tan, C. Teles, F. Noronha

4:20 I&EC 36. Understanding and design of metal based catalysts. **Y. Wang**

4:50 Concluding Remarks.

Section C
Loews New Orleans Hotel
Louisiana II

I&EC International Fellow: Symposium in honor of Shahidah Mohd Shariff

A.S. Hussain, *Organizer, Presiding*
1:00 Introductory Remark.

1:05 I&EC 37. Unlocking new opportunities: From seeing the unseen to fueling world champions. A.S. Hussain, M. Abai, **S. M Shariff**

1:30 I&EC 38. Of empowering talents & driving innovations. **M. Abai**, A.S. Hussain, S. M Shariff

1:45 I&EC 39. Foam-assisted water alternating gas (FAWAG) formulation design: Efficiency and sustainability. I.C. Chai, V. Hon, **P. A Hamid**

2:05 I&EC 40. Phase behavior study for carbon dioxide rich natural gas: Carbon dioxide solids and hydrate formation. **A. Md Jalil**, N. Othman, Z. Kassim, R. Salihuddin, A. Abu Seman, F. Rahman, M. Mat Isa

2:20 Intermission.

2:35 I&EC 41. Sand agglomeration in oil & gas reservoirs: Chemistry, experiments and simulations. **O.K. Matar**, R. Lee, A. Shaffee, P. Luckham

2:55 I&EC 42. Exploring wax precipitation in crude oils through diffusion ordered spectroscopy nuclear magnetic resonance combined with molecular dynamics simulations. **S. Shahruddin**, G. Jiménez-Serratos, G.J. Britovsek, O.K. Matar, E. Muller

3:10 I&EC 43. Mercury removal from natural gas condensate using solid supported ionic liquid. Y. Kuah, **S. Bin Mohd Azam Shah Wong**, A. Bin Hassan, N. Binti A Manan, M. Bin Ishak, S. Binti M Shariff, A. Bin A Rahman, M. Bin A Hamid

3:30 I&EC 44. Development of PETRONAS own drilling fluid, MG3DF. A. Hassan, **M. Abai**, J. Basar, S. Lee, A. Abidin, H. M Ali, S. Binti M Shariff

3:45 I&EC 45. From waste to wealth: Carbon fixation using gas fermentation. **S. Simpson**

4:05 I&EC 46. Ethylene oligomerisation beyond Schulz-Flory distributions. **G.J. Britovsek**, A.K. Tomov, E. Muller, O.K. Matar, S. Shahruddin, C. Young

4:25 I&EC 47. Mannich reactions catalyzed by sulfonate for the construction of bioactive organic moieties. **C.D. Wilfred**, J. Leveque, S. Sardar

4:40 I&EC 48. Tailoring hydrocarbon composition and functional groups for fuel efficiency. **M. Chan**, C.A. Muthiah

4:55 Concluding Remarks.

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY MORNING

Section A
Loews New Orleans Hotel
Louisiana I

I&EC Early Career Fellow: Symposium in honor of Beata Kilos

D.G. Barton, E. Nikolla, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 49. Site and structural requirements for stabilization of transition states for oligomerization and hydrogen transfer reactions on solid acids. M. Sarazen, **E. Iglesia**

8:50 I&EC 50. Niobium: A love story. N. Thornburg, A. Ardagh, E. Taw, **J.M. Notestein**

9:20 I&EC 51. Mechanisms, active intermediates, and descriptors for epoxidation rates and selectivities on dispersed early transition metals. **D. Flaherty**, D. Bregante, A. Johnson, A. Patel

9:50 Intermission.

10:10 I&EC 52. Catalytic partial oxidation of olefins: A functional assessment inspired by mechanistic and kinetic analysis. **A. Bhan**

10:40 I&EC 53. Design of high activity supported catalysts for olefin metathesis based on dispersed metal oxides. **S.L. Scott**

11:10 I&EC 54. Reaction mechanism and the nature of the active site for standard selective catalytic reduction of NOx on Cu/SSZ-13 zeolites. **F. Ribeiro**, W. Delgass, R. Gounder, J.T. Miller, W.F. Schneider, A. Yezerets, A.A. Parekh, C. Paolucci, I. Khurana, J. Albarracin, J.R. Di Iorio, A.J. Shih

11:40 Concluding Remarks.

Section B
Loews New Orleans Hotel
Feliciana East

E.V. Murphree Award in Industrial and Engineering Chemistry: Symposium in honor of Linda J. Broadbelt

Cosponsored by WCC
D.J. Klinke, *Organizer*
H. Kung, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 I&EC 55. The role of atomistic modeling in precursor design for nanostructured film deposition. **A. Adamczyk**

9:05 I&EC 56. Structured polymer colloids via constrained volume self-assembly. **R.D. Priestley**

9:35 I&EC 57. Withdrawn.

10:05 Intermission.

10:25 I&EC 58. Coupling of mass transfer and chemical kinetics during co-pyrolysis of cellulose and high-density polyethylene. M. Nallar, **H. Wong**

10:55 I&EC 59. On the use of analytical solutions and dimensionless numbers to guide polymerization system understanding and design. **I. Konstantinov**, C. Villa, T. Karjala, P. Jain

11:25 I&EC 60. Acrylate monomer reactivity and polymer architecture models for improved structure/property relationships. **S.G. Arturo**, I. Konstantinov, G. Zhang, V. Regatte, H. Gao, L.J. Broadbelt

Molecules that Changed the World
Sponsored by YCC, Cosponsored by HIST and I&EC

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Rafael Luque
Sponsored by CELL, Cosponsored by ENVR and I&EC

Industrial Innovations in Polymer Science
Sponsored by POLY, Cosponsored by I&EC

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY AFTERNOON

Section A
Loews New Orleans Hotel
Louisiana I

I&EC Early Career Fellow: Symposium in honor of Beata Kilos

D.G. Barton, E. Nikolla, *Organizers*
A. Kulkarni, L. San Miguel, *Presiding*

1:00 Introductory Remarks.

1:05 I&EC 61. Influence of shale gas on industrial catalyst research. **D.G. Barton**

1:35 I&EC 62. Oxygen electrocatalysis using layered mixed metal oxides. **E. Nikolla**

2:05 I&EC 63. Completing the cycle: How field experience informs catalyst design and process improvement. **W. Vining**, W.J. Hizny, M.T. Buelow, J. Lapadula, P. Tran

2:35 Intermission.

2:55 I&EC 64. Molten salt catalysis forming OH radicals from oxygen and water and their reactions with hydrocarbons. **K. Takanabe**

3:25 I&EC 65. Teaching an old dog new tricks: Size-dependent photocatalytic activity of supported vanadium oxide species. B. Kortewille, I.E. Wachs, N. Cibura, G. Bacher, O. Pfingsten, M. Muhler, **J. Strunk**

3:55 I&EC 66. Acceptorless dehydrogenative coupling of ethanol over bulk MoS_2 and spectroscopic structure-function correlations . **L.R. McCullough**, E.S. Cheng, A.A. Gosavi, B.A. Kilos, D.G. Barton, E. Weitz, H. Kung, J.M. Notestein

‡*Cooperative Cosponsorship*

4:25 Concluding Remarks.

Section B
Loews New Orleans Hotel
Feliciana East

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Fengqi You
Cosponsored by CELL
D. Garcia, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 I&EC 67. Synthesis and characterization of functional metal–organic framework materials. **O.K. Farha**

1:30 I&EC 68. Engineering nanostructured materials to measure water stress in plants. **A. Stroock**, S. Zhu, P. Jain

1:55 I&EC 69. Capturing and separating ammonia with metal-organic framework materials. **J.T. Hupp**, M. Rimoldi, A. Howarth, O. Farha

2:20 I&EC 70. Computational modeling of nanoporous materials for precombustion CO_2 capture and hydrocarbon separation. **Y.G. Chung**, D. Gomez Gualdron, P. Bai, J.I. Siepmann, R. Snurr

2:45 Intermission.

3:00 I&EC 71. Engineering and optimizing the co-assembly of nanoparticle alloys via molecular simulations. **F. Escobedo**

3:25 I&EC 72. Modeling of metal-organic frameworks as tunable adsorbents for separations. K.T. Leperi, Y.G. Chung, B. Bucior, F. You, **R. Snurr**

3:50 I&EC 73. Chemical looping oxidative dehydrogenation for ethylene production with a smaller carbon footprint. **F. Li**

4:15 I&EC 74. Multi-scale life cycle analysis and optimization for sustainable chemistry & engineering. **F. You**

4:40 Concluding Remarks.

Industrial Innovations in Polymer Science
Sponsored by POLY, Cosponsored by I&EC

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
C.W. Abney, *Organizer*
8:00–10:00

26, 42, 46, 58, 68. See previous listings.

94, 103, 110-111, 120, 122, 125, 128, 135, 137, 140, 144. See subsequent listings.

TUESDAY MORNING

Section A
Loews New Orleans Hotel
Louisiana I

I&EC Early Career Fellow: Symposium in honor of Beata Kilos

D.G. Barton, E. Nikolla, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 75. The role of metal cations in the activation of C-H bonds in organic compounds. **A.T. Bell**

8:50 I&EC 76. Maximizing efficiencies of photocatalytic water splitting by engineering interfaces in multi-component photocatalysts. **S. Linic**

9:20 I&EC 77. Activity and speciation of supported pincer-ligated iridium catalysts in continuous-flow gas phase alkane dehydrogenation. **F.E. Celik**, B. Sheludko, A.S. Goldman

9:50 Intermission.

10:10 I&EC 78. Identity of reactive hydrogen species and their transfer during the hydrogenation of aldehydes and ketones. **Y. Chin**, J. Shangguan, Z. Wu

10:40 I&EC 79. Catalytic oxidative esterification of aldehydes to esters with air over supported Pd catalysts promoted with Bi or Sb. A. Kirilin, **W. Lee**, V.J. Sussman, M. Bashir, T. Calverley, H. Clements, J. Kang, L. Bogan

11:10 I&EC 80. Vapor phase ethanol carbonylation over supported rhodium catalysts. **S. Yacob**, B.A. Kilos, D.G. Barton, J.M. Notestein

11:40 Concluding Remarks.

Section B
Loews New Orleans Hotel
Feliciana East

I&EC Fellow: Symposium in honor of Dave Mackowiak: ACTP

C.P. Nicholas, *Organizer, Presiding*
8:00 Introductory Remarks.

8:05 I&EC 81. Methods for characterizing acidity on solid catalysts. **R. Miller**, T. Mezza

8:30 I&EC 82. Acetylene hydrogenation catalyst testing. **G. Barbay**, M. Brayden

8:55 I&EC 83. Not all Nitrogens are equal: Contribution of peripheral versus internal amines to the observed reactivity and capture properties of melamine dendrons on SBA-15. **Y. Lou**, D.F. Shantz

9:20 Intermission.

9:35 I&EC 84. From proof-of-principle to commercialization of Honeywell Ecofining™ and UOP Renewable Jet Fuel Process™ technologies. **P.T. Barger**

10:00 I&EC 85. Honeywell's low climate impact fluorocarbons. **T. Stith**

10:25 I&EC 86. From exploratory research to proof of principle: Laboratory testing at Honeywell UOP. **D. Mackowiak**

10:50 Award Presentation.

11:00 I&EC 87. New process technology for conversion of acetic acid to ethanol and acrylic acid. **R.D. Gillespie**, J. Chapman, C. Peterson, D. Lee, S. Mueller

11:25 Concluding Remarks.

2018 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Ning Yan
Sponsored by CELL, Cosponsored by ENVR and I&EC

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY AFTERNOON

Section A
Loews New Orleans Hotel
Louisiana I

I&EC Early Career Fellow: Symposium in honor of Beata Kilos

D.G. Barton, E. Nikolla, *Organizers*
A. Kulkarni, L. San Miguel, *Presiding*

1:00 Introductory Remarks.

1:05 I&EC 88. MOF mediated synthesis of Fischer-Tropsch catalysts: Thinking out of the box. **V. Santos**, T. Wezendonk, A. Chojecki, J. Gascon, F. Kapteijn, M. Ruitenbeek, G. Meima

1:35 I&EC 89. Mechanistic consequences of Cu ion mobility in zeolites for the selective catalytic reduction of nitrogen oxides with ammonia. **R. Gounder**

2:05 I&EC 90. Elucidating the mechanism for the catalytic hydrodeoxygenation of phenols. B. Jake, A. Hensley, B. Wong, D. Mei, Y. Wang, **J. McEwen**

2:35 Intermission.

2:55 I&EC 91. Advanced zeolite catalysis technologies for clean air. **B. Moden**, H. Li

3:25 I&EC 92. Hydroprocessing catalyst system design for tailoring crude oils characterized by advanced analytical techniques. M. Hurt, **B. Zhan**

3:55 I&EC 93. Untraveled roads to familiar destinations: exploring new pathways to produce classic chemicals. **B.A. Kilos**, L. Luo, D.G. Barton, J. Kang, B. Stears, A. Malek, W. Lee, C. Yang, J.M. Notestein

4:35 Concluding Remarks.

Section B
Loews New Orleans Hotel
Feliciana East

Water Purification for a Sustainable Future

G.M. Geise, *Organizer*
S.M. Mahurin, *Organizer, Presiding*
1:00 Introductory Remarks.

1:05 I&EC 94. Wastewater treatment by catalytic wet air oxidation process over a Tunisian clay pillared with Al-Fe. **G. Lafaye**, H. Sassi, H. Ben Amor, M. Jeday, J. Barbier Jr

1:35 I&EC 95. Advanced adsorbents for the extraction of uranium from seawater. **R.T. Mayes**

2:05 I&EC 96. Electrically enhanced adsorption and green regeneration for fluoride removal using $Ti(OH)_4$-loaded activated carbon electrodes. Y. Li, C. Zhang, Y. Jiang, **T. Wang**

2:35 Intermission.

2:50 I&EC 97. Membrane-based water desalination: From graphene to porous carbon. **S.M. Mahurin**, I. Vlassiouk, S. Dai

3:20 I&EC 98. Structure/property relationships in polymer membranes for water purification and energy applications. **G.M. Geise**

3:50 I&EC 99. The influence of graft-polymer chain length on uranium binding mode: Identifying the origins of emergent phenomena. **C.W. Abney**, L. Earl

4:20 Concluding Remarks.

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

General Posters

C.W. Abney, *Organizer*
6:00–8:00

I&EC 100. Functionalized nanocrystalline cellulose sorbents for efficient carbon dioxide (CO_2) capture at elevated temperatures. **A.C. Dassanayake**, C. Gunathilake, R.S. Dassanayake, N. Abidi, M. Jaroniec

I&EC 101. Synthesis carbide from supercritical CO_2-ethanol extraction residues of powder river basin coal. **K. Sun**, X. He, M. Tang, M. Fan

I&EC 102. Carbon fiber formation from supercritical carbon dioxide extraction tar/PAN with $Bi(NO_3)_3$ as photocatalyst. **X. He**, M. Tang, K. Li, F. Liu, K. Sun, M. Fan

I&EC 103. Improved hybrid adsorption-absorption method to capture carbon. **S. Yan**

I&EC 104. Amidine- and imidazole-based ionic liquids for CO_2 capture. **C. Do-Thanh**, J.A. Schott, S.M. Mahurin, S. Dai

I&EC 105. The stability of $V(acac)_3$ in the presence of ionic liquids. **J. Lee**, J. Kim, J. Lee

I&EC 106. Property of piperidinium-based ionic liquids containing nitrile group on cation. **C. Oh**, S. Park, J. Lee

I&EC 107. Prepared self-assembled ionogels and their ion transfer properties. **S. Lee**, S. Park, J. Lee

I&EC 108. Preparation of porous carbons using polysaccharides as electrodes of EDLC. **S. Park**, S. Lee, J. Lee

I&EC 109. Porous carbon electrodes for supercapacitor prepared by a soft template method. **J. Kim**, J. Lee, J. Lee

I&EC 110. Comparative study of wet vs dry biochar ozonization on oxygenation of biochar surface and dissolved organic carbon. A. Pullin, K. Blowe, D. Arrington, G. Kharel, S. Abate, A. Sika, S. Kumar, **J.W. Lee**

I&EC 111. Surface enhanced Raman spectroscopy of catalytically active $AuNP/TiO_2$ composites. **A. Prokofjevs**, M. Kung, H. Kung

I&EC 112. New odor control technology for drainage system. S. Wong, L. Luk, **M. Arjona Alonso**, W. Han, K. Yeung

‡*Cooperative Cosponsorship*

WEDNESDAY MORNING

Section A
Loews New Orleans Hotel
Louisiana I

General Papers

C.W. Abney, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 113. Preparing the industrial workforce: The role of operator in research and in production. **F.K. Wood-Black**

8:25 I&EC 114. Single-walled carbon nanotube-based chemiresistive sensors for food and agriculture. **J.M. Schnorr**, J. Goods, T.M. Swager

8:45 I&EC 115. Rynaxypyr® insecticide: A case study in the discovery through commercialization of modern crop protection chemicals. **G.P. Lahm**, T.P. Selby, T.M. Stevenson, D. Cordova

9:05 Intermission.

9:25 I&EC 116. Fabrication of free-standing, superomniphobic films for effective chemical shielding. **H. Vahabi**, W. Wang, S. Movafaghi, A. Kota

9:45 I&EC 117. Developments in monitoring continuous reactions by ruggedized, online benchtop NMR. **S. Riegel**, J. Araneda

10:05 I&EC 118. Novel measurement of shear strength using thermal strain. **G. Kim**

10:25 Intermission.

10:45 I&EC 119. Antimicrobial non-irritant wound dressings through N-halamine surface modification. **B. Demir**, S.D. Worley, R. Broughton, T. Huang

11:05 I&EC 120. Insights into interfacial behaviors for the isobutane alkylation with C4 olefins using ionic liquids as catalyst. **W. Sun**, W. Zheng

11:25 I&EC 121. Acid-catalyzed synthesis of trioxane in aprotic media. **W. Ma**, Y. Hu

11:45 Concluding Remarks.

Section B
Loews New Orleans Hotel
Feliciana East

Inaugural Joint Symposium of the Separation Science Subdivisions
Cosponsored by ANYL
C. Rimmer, *Organizer*
G.A. Fugate, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 122. Physical separations of rare earth elements from coal and coal by-products. **Y. Soong**, R. Lin, B. Howard, E. Roth, T. Bank, E.J. Granite

8:30 I&EC 123. Determination of the halogen content of polymers and electronics using combustion Ion chromatography. **B. Huang**, J. Rohrer

8:55 I&EC 124. Closing nuclear fuel cycle With ALSEP process: Hot multistage demonstration. **A. Gelis**, A. Breshears, M. Brown, P. Kozak

9:20 Intermission.

9:40 I&EC 125. Aminopolymer synthesis, characterization, and use in composite sorbents for CO_2 capture. **M. Sarazen**, C.W. Jones

10:30 I&EC 126. Efficient and selective extraction of $^{99m}TcO_4^-$ from aqueous media using hydrophobic deep eutectic solvents. **T.E. Phelps**, N. Bhawawet, G.A. Baker, S.S. Jurisson

10:55 I&EC 127. High temperature size exclusion chromatography measurements of polyolefins with precise control of branch frequency and branch length . **S.V. Orski**, W. Farrell, K. Beers

11:20 Concluding Remarks.

Section C
Loews New Orleans Hotel
Louisiana II

ACS Pharma Roundtable: Innovative Green Processing Technology & Chemistry

M.E. Kopach, *Organizer*
D. Entwistle, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 128. Synthetic transformation employing continuous flow technologies and green solvent systems. **C.L. Liotta**, P. Pollet, S.A. France

8:45 I&EC 129. Small volume continuous production of a clinical candidate through a green lens. **K. Cole**

9:25 I&EC 130. Lowering the dose for critical medicines by improving pharmacokinetics: A new approach to improving global medicines access. **J.M. Fortunak**, F.E. Nytko, T. Ellison

10:05 Intermission.

10:25 I&EC 131. Strategies and methods for the synthesis of neuroactive disulfide-linked peptides. **J.L. Stockdill**

11:05 I&EC 132. Enabling technologies applied to accelerating oncology projects in a sustainable manner. **P. Richardson**

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

WEDNESDAY AFTERNOON

Section A
Loews New Orleans Hotel
Louisiana I

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde
Cosponsored by INOR‡
P.J. Pauzauskie, *Organizer*
R.M. Richards, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 I&EC 133. Nanostructured materials with unique catalytic properties. **R.M. Richards**

1:35 I&EC 134. From fundamental molecular recognition to practical applications. **C.B. Aakeroy**

1:55 I&EC 135. Solvated metal atom dispersion and digestive ripening – duo *par excellence* for diverse nanostructured materials. **B.R. Jagirdar**

2:15 I&EC 136. Single molecule pathways to a better understanding of mass transport in nanostructured materials. **D.A. Higgins**, T. Ito, R. Kumarasinghe, H. Xu

2:35 Intermission.

2:45 I&EC 137. Mesoporous silica-templated metal, metal oxide, and metal carbide/nitride catalysts with unique structures and properties for catalytic reactions relevant to biomass upgrading. **S. Gage**, B.G. Trewyn, S. Pylypenko, R.M. Richards

3:05 I&EC 138. Bimetallic nanoclusters/chiral polymers in catalytic asymmetric oxidation. **B. Hao**, K. Apley, D.H. Hua

3:25 I&EC 139. Synthesis, characterization, and catalytic activity of ionic liquid templated mesoporous zirconia. **J. Roach**, A. Spink, D.S. Heroux

Section B
Loews New Orleans Hotel
Feliciana East

Inaugural Joint Symposium of the Separation Science Subdivisions
Cosponsored by ANYL
C. Rimmer, *Organizer*
G.A. Fugate, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 I&EC 140. Hydrogen sulfide capture using amine-modified mesoporous adsorbents. **C. Okonkwo**

1:30 I&EC 141. Monte Carlo simulations of separation processes with solid mass separating agents: Molecular-level insights and materials design. **J.I. Siepmann**

1:55 I&EC 142. Molecular simulation insights on Xe/Kr separation in a set of nanoporous crystalline membranes. R. Anderson, B. Schweitzer, T. Wu, M.A. Carreon, **D. Gomez Gualdron**

2:20 I&EC 143. Odor-control technology for H_2S malodor problem in dewatered sludge from chemically-enhanced primary treatment process. **M. Arjona Alonso**, K. Cheng, W. Han, K. Yeung

2:45 Intermission.

3:05 I&EC 144. Surface-functionalized nanomaterials for separation processing of crude and aqueous fractions of biooils. **M.Z. Hu**, M. Lu

3:30 I&EC 145. Optical Technique for In Situ Measurement of Concentration Polarization in Direct Contact Membrane Distillation. **O.R. Lokare**, P. Ji, G. Dutt, R.D. Vidic

3:55 I&EC 146. Optical probes of liquid-liquid extraction speciation and kinetics in real-time. **M.P. Jensen**, G. Picayo, M.A. Eddy

4:20 Concluding Remarks.

Section C
Loews New Orleans Hotel
Louisiana II

ACS Pharma Roundtable: Innovative Green Processing Technology & Chemistry

M.E. Kopach, *Organizer*
D. Entwistle, *Organizer, Presiding*

1:00 I&EC 147. Benchmarking green chemistry adoption by the global pharmaceutical supply chain. **B.W. Cue**, V. Veleva

1:40 I&EC 148. Streamlined functionalization of pyridines, diazines and pharmaceuticals. **A. McNally**

2:20 Intermission.

2:40 I&EC 149. Advanced engineered biocatalysts for sustainable pharmaceutical manufacture. **D. Entwistle**

3:20 I&EC 150. Evolution of a chemical process (from the laboratory and beyond). **J.D. Brown**

4:00 Concluding Remarks.

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

THURSDAY MORNING

Section A
Loews New Orleans Hotel
Louisiana I

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde
Cosponsored by INOR‡
P.J. Pauzauskie, *Organizer*
R.M. Richards, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC 151. Titania nanoclusters supported on siliceous mesoporous materials for photocatalytic water splitting. **R.T. Koodali**

8:35 I&EC 152. Rapid heat-up synthesis of quantum dots with color-tunable photoluminescence. **E.J. McLaurin**

8:55 I&EC 153. Rapid colloidal nanoparticle synthesis. **V. Chikan**

9:15 I&EC 154. Theoretical investigation of the electronic structure and stability for doped Au_{25} clusters. **F. Alkan**, A.R. Munoz Castro, C.M. Aikens

9:35 Intermission.

9:45 I&EC 155. pH-Dependent surface chemistry of metal oxide nanoparticles in biological and environmental media. **V.H. Grassian**

10:15 I&EC 156. High commercial value carbon nanomaterials from biomass for energy storage. **Z. Li**

10:35 I&EC 157. Liquid biopsies for early stage solid tumors. **S.H. Bossmann**, M. Kalubowilage, O. Covarrubias-Zambrano, A.P. Malalasekera, H. Wang, S.O. Wendel, G. Zhu, D.L. Troyer

Section B
Loews New Orleans Hotel
Feliciana East

Separation Science & Technology in the Medical Cannabis & Hemp Industry
Cosponsored by CHAS
E.M. Pryor, *Organizer*
J.W. King, *Organizer, Presiding*
E. Pryor, *Presiding*

8:00 Introductory Remarks.

8:05 I&EC 158. Grinding: The delicate dance between optimization and repetition to control extraction outcomes. **M. Roggen**, **B. Schubmehl**

8:25 I&EC 159. Scaling the purification of cannabis extracts: High-throughput strategies for the isolation of cannabinoids and remediation of contaminants. **E. Miler**, J. Thompson

‡*Cooperative Cosponsorship*

8:45 I&EC 160. Harnessing the advantages of SFC for next generation cannabinoid products. **B.G. Reid**

9:05 I&EC 161. Microdetermination of cannabinoid solubilities in gaseous solvent mixtures. **R.B. Murphy**, R. Liu, A. Martinez, D. Grigoreva, L. Snyder, C. Camara

9:25 I&EC 162. Supercritical fluids manufacturing of cannabidiol (CBD) and other cannabinoids from *Cannabis sativa* following cGMP guidelines of the US FDA. **T. Castor**

9:45 Intermission.

10:00 I&EC 163. Different operation conditions and regimes in supercritical extraction of cannabinoids: The role of co-solvent at pilot scale. **L.J. Rovetto**, **N.V. Aieta**

10:20 I&EC 164. PLOT-cryoadsorption: Determination of cannabinoid vapor pressure. **T. Bruno**, **T. Lovestead**

10:40 I&EC 165. Processing industrial hemp-derived CBD extract: From crude oil to finished products. **A. Pham**

11:00 I&EC 166. Obtaining a plant sample with low cannabinoid content using supercritical fluid extraction (SFE). **A.C. Gallo Molina**, F. Parada, W. Garzón, J.A. Martínez

11:20 I&EC 167. Industrial-scale cannabis indica drug processing. **J. Yeary**

11:40 I&EC 168. Design and optimization of cannabinoid and terpene enrichment processes by chemical engineering capstone design engineering teams at the University of Alberta. **J.W. King**, M. Jamieson

THURSDAY AFTERNOON

Section A
Loews New Orleans Hotel
Louisiana I

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde
Cosponsored by INOR‡
R.M. Richards, *Organizer*
P.J. Pauzauskie, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 I&EC 169. Copper-mediated synthesis and optoelectronic trapping of ultra-high aspect ratio palladium nanowires. **P.J. Pauzauskie**, J. Hanson, M. Lim, L. Vandsburger, P. Roder, X. Zhou, B. Smith, F. Ohuchi

1:35 I&EC 170. High-performance electrical energy storage based on hierarchical hybrid structures. **J. Li**

1:55 I&EC 171. Materials electrochemistry in rechargeable alkali metal ion batteries. **F. Lin**

2:15 I&EC 172. Low valent coordination complexes of nickel for the activation of chalcogens. **C.G. Riordan**, J. Wallick

2:35 Intermission.

2:45 I&EC 173. Structure-function relationships at the molecular level: Controlling the secondary coordination sphere. **A. Borovik**

3:05 I&EC 174. Stable rhodium single-site catalyst embedded in dendritic nanospheres. J. Tian, D. Yang, J. Wen, A. Filatov, Y. Liu, A. Lei, **X. Lin**

3:25 I&EC 175. Stabilizing Ni-rich layered cathode materials via elemental substitution for high energy lithium batteries. **J.D. Steiner**, J. Walsh, B. Zydlewski, F. Lin

INOR

Division of Inorganic Chemistry

S. Koch and N. Radu, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Homogeneous Catalysis for Applied Organic Synthesis (see *CATL*, Mon, Tue)

Innovative Chemistry & Materials for Electrochemical Energy Storage (see *ENFL*, Sun, Mon, Tue, Wed)

Carbon Dioxide Conversion & Artificial Photosynthesis (see *ENFL*, Sun, Mon, Tue)

Actinide Complexes & Nanoclusters (see *NUCL*, Sun, Mon, Tue)

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium (see *PROF*, Sun, Mon)

Radiopharmaceutical Chemistry (see *FLUO*, Tue, Wed, Thu)

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 345

Synthetic Chemistry Addressing Challenges in Energy & the Environment
Cosponsored by CATL and WCC
L.A. Berben, A. De Bettencourt Dias, A.L. Prieto, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 INOR 1. Synthesis and characterization of the Zintl phase $Yb_{2-x}Eu_xCdSb_2$ for direct thermal to electrical energy conversion. **S. Kauzlarich**

8:55 INOR 2. Mössbauer spectroscopic insights into the electronic structure and mechanism of bio-inspired iron complexes. **C.V. Popescu**, P. Ghosh, S. Ding, M.Y. Darensbourg, M.B. Hall

9:15 INOR 3. The synthesis and characterization of metal organic frameworks for CO_2 utilization. J. Zhu, P. Usov, **A.J. Morris**

9:35 Intermission.

9:45 INOR 4. Obtaining white light from layered perovskites. M.D. Smith, A. Jaffe, E. Dohner, A. Lindenberg, **H. Karunadasa**

10:05 INOR 5. Linear and star block copolymers derived from biorenewable resources as adsorbents for waste water remediation. **A.M. Balija**, K. Bernhardt, K. Moore

10:25 INOR 6. New trimetallic assemblies for solar energy conversion: combining new light absorbers with new catalysts. **C. Turro**, W.T. Kender, K.R. Dunbar

10:45 Intermission.

10:55 INOR 7. Developing a mild and modular route to chemically modified electrodes for photoelectrochemical cells. **J.Y. Yang**

11:15 INOR 8. Use of peptoids for molecular recognition of contaminants in water. **A.A. Fuller**, K.M. Tenorio, J. Huber, K. Dowell, S. Hough

11:35 INOR 9. Re-wiring biological hydrogen production. **A. Parkin**

Section B
Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, H. Zhou, *Organizers*
S. Ma, *Organizer, Presiding*
B. Wang, *Presiding*

8:30 Introductory Remarks.

9:20 INOR 10. MOF design to applications: Impact of pore system control on gas separations and storage. **M. Eddaoudi**

9:50 INOR 11. polyMOFs: Bridging the polymer-MOF materials gap. **S. Cohen**, Z. Zhang, S. Ayala, G. Schukraft

10:20 Intermission.

10:30 INOR 12. The organic secondary building unit: π-Stacking interactions define topology in MOFs. **M. Dinca**, S. Park, L. Xie

11:00 INOR 13. Electrically conductive coordination networks. **H. Kitagawa**

11:30 INOR 14. Metal-organic frameworks applications in the face of increasing demand for novel electronic materials to advance special purpose technologies. **J. Ornstein**, R. Ozdemir

Section C
Ernest N. Morial Convention Center
Room 343

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak

J.S. Figueroa, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR 15. Role of uranium–arene bonding in H_2O reduction catalysis. **K. Meyer**

9:00 INOR 16. Excited states of new bimetallic complexes for solar energy applications. **C. Turro**, T.J. Whittemore, C. Xue, T.A. White, H.J. Sayre

9:25 INOR 17. Elucidating the mechanism of CO_2 reduction to CO by group 6 $M(CO)_6$ species using infrared spectroelectrochemisty and quantum chemistry. **K.A. Grice**, C. Saucedo, M. Groenonboom, J. Nganga, A.M. Angeles Boza, J.A. Keith

9:50 INOR 18. Organic mixed valence compounds and Kekulé diradicaloids derived from CAACs. **G. Bertrand**

10:15 INOR 19. Polypyridyl electrocatalysts for the reduction of CO_2. L. Lieske, **C.W. Machan**

10:40 Intermission.

11:00 INOR 20. Running the alphabet from A(-frames) to Z(-schemes) with hydrogen. **R. Eisenberg**

11:25 INOR 21. Second-sphere coordination assists metal-halogen bond photoactivation. **D.G. Nocera**, S. Hwang, D. Gygi

11:50 INOR 22. From ceiling to fluorine: Stable metal heptafluoroisopropyl complexes and transfer reagents. N.O. Andrella, K. Liu, M. Vasiliu, D.A. Dixon, **R. Baker**

Section D
Ernest N. Morial Convention Center
Room 352

ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer

S.N. Brown, C.T. Saouma, *Organizers*
J.J. Warren, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR 23. Interfacial proton-coupled electron transfer: Interplay between experiment and theory. **S. Hammes-Schiffer**

8:55 INOR 24. Identifying proton-coupled electron transfers that give rise to potential-pK_a relationships in catalysis. **J.L. Dempsey**, E. Rountree, B.D. McCarthy

9:15 INOR 25. Mechanisms and distance-dependence of proton-coupled electron transfer. **L. Hammarstrom**

9:35 INOR 26. Hydrogen atom transfer reactions of bis(iminosemiquinonato) palladium(II) and -platinum(II): Thermodynamic and kinetic coupling. **S.N. Brown**, K.M. Conner, A.C. Arostegui, D.D. Swanson

9:55 INOR 27. Investigating concerted proton-electron transfer with base-appended radical cations. E.A. Welker, D.J. Robinson, B.L. Tiley, C.M. Sasaran, M. Vettleson, N.T. Fretz, J.J. Geruntho, M.A. Zuchero, W. Tong, R.A. Richards, F.M. Simpson, S. Stoll, J. Wolbach, **I.J. Rhile**

10:15 Intermission.

10:25 INOR 28. Examining the effects of structural modifications on explosive sensitivity. **V. Manner**, M. Cawkwell, E. Kober, T. Myers, J. Yeager, G. Brown, H. Tian

10:45 INOR 29. Metal complexes of "two-story" calix[6]arene ligands: Structure and reactivity. **D.E. Over**, G. De Leener, N. Le Poul, F. Topić, K.T. Rissanen, Y.F. Le Mest, I. Jabin, O. Reinaud

11:05 INOR 30. Sterically undemanding pincer ligands: Reactions of iridium complexes. **D.M. Heinekey**, T. Lekich, B. Gary, S.M. Bellows, T.R. Cundari

11:25 INOR 31. Sulfuric acid catalyzed cyclohexylbenzene hydroperoxide cleavage: effects of reaction medium and mechanistic implications. **K. Wang**, R. Garcia

‡*Cooperative Cosponsorship*

Section E
Ernest N. Morial Convention Center
Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Roman-Leshkov, *Organizer*
Y. Surendranath, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 INOR 32. Hydrocarbon separations in metal-organic frameworks. J. Bachman, M. Kapelewski, M.I. Gonzalez, D. Reed, E.D. Bloch, Z. Herm, J.A. Mason, **J.R. Long**

8:40 INOR 33. Advanced porous organic polymers for environmental remediation. **S. Ma**

9:10 INOR 34. Postsynthetic metal exchange in pincer MOFs. **C.R. Wade**, A.A. Kassie

9:40 INOR 35. Bioinspired sponges: Design principles for metal-organic frameworks-enzymes composite. **O.K. Farha**

10:10 Intermission.

10:30 INOR 36. Strategies for incorporating p-block element catalysts inside MOFs for reductions and oxidations.. B. Tahmouresilerd, P. Larson, **A.F. Cozzolino**

11:00 INOR 37. Metal-organic frameworks as flasks: Chromophore photophysics in a confined environment. **N.B. Shustova**, E. Dolgopolova, A.M. Rice

11:30 INOR 38. Withdrawn

Section F
Ernest N. Morial Convention Center
Room 354

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Cosponsored by WCC
J.S. Martinez, *Organizer*
M. Haygood, *Presiding*

8:30 Introductory Remarks.

8:40 INOR 39. Siderophore production and quorum sensing in the marine bacterium *Vibrio Harveyi*. D.L. McRose, **F. Morel**

9:05 INOR 40. Iron recycling in marine systems: Of microbes and molecules. **K.A. Barbeau**

9:30 INOR 41. Alkane oxidizing enzymes in the marine environment: What we can learn from integrating biochemistry, microbiology, and omic databases. **R.N. Austin**

9:55 INOR 42. Siderophores in a symbiotic system. **M. Haygood**, H. Naka

10:20 Intermission.

10:40 INOR 43. Abundant mesopelagic metalloenzymes in the Pacific oxygen minimum zone. **M. Saito**, M.R. McIlvin, D.M. Moran, A. Santoro, C. Dupont, C. Lamborg, P. Rafter

11:05 INOR 44. Redox chemistry and mussel adhesion. **H. Waite**

11:30 INOR 45. Mechanistic investigations of manganese(IV) oxide biomineralization catalyzed by a multicopper oxidase complex. **B.M. Tebo**, C. Romano, A. Soldatova, M. Zhou, A.C. Dohnalkova, L. Kovarik, L. Tao, T.A. Stich, Y. Song, V.H. Wysocki, L. Pasa-Tolic, W.H. Casey, R. Britt, T.G. Spiro

11:55 INOR 46. Solution and (nano) particulate chemistry within the dynamic mixing zone of the first 2 meters of hydrothermal vent orifices. **G.W. Luther**, E.R. Estes, A. Findlay, M. Yucel, A. Gartman, R. Rosas, N.R. Coffey, V.E. Oldham, T.J. Shaw, J. Ferry, M.c. Dias, B.M. Tebo

Section G
Ernest N. Morial Convention Center
Room 210

Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/ Denitrification Reactions

K.M. Lancaster, *Organizer*
N. Lehnert, *Organizer, Presiding*

8:30 INOR 47. Nitrite-ammonia expressway, with no stop at dinitrogen. **P.M. Kroneck**

9:00 INOR 48. Evolution and modularity of ammonia oxidation pathways. L.Y. Stein, **M.G. Klotz**

9:30 INOR 49. Evaluating the mechanism of NO reduction in a flavodiiron nitric oxide reductase model complex. **C. White**, N. Lehnert

9:50 INOR 50. Nitrous oxide reduction mediated by a nucleophilic nickel(II) sulfide. **T.W. Hayton**

10:20 Intermission.

10:30 INOR 51. Structure and function of particulate methane monooxygenase, an ammonia monooxygenase homolog. **A.C. Rosenzweig**

11:00 INOR 52. Synthetic copper-sulfide models of Cu_z with activity towards N_2O and other small molecules. B. Johnson, S. Bagherzadeh, S. Rathnayaka, C. Hsu, **N.P. Mankad**

11:30 INOR 53. Revision by enzymology of bacterial ammonia oxidation. **J.D. Caranto**

11:50 INOR 54. Probing mechanisms of nitrous oxide generation in a denitrifying polyphosphate accumulating bacteria enrichment culture. H. Gao, Y. Mao, T. Zhang, **G. Wells**

Section H
Ernest N. Morial Convention Center
Room 211

Undergraduate Research at the Frontiers of Inorganic Chemistry

C. Nataro, L.A. Watson, *Organizers*
K.L. Stone, *Presiding*

8:30 Introductory Remarks.

8:40 INOR 55. Schiff-base vanadium(V) catecholate complexes and their interactions with a model membrane interface. S.M. Petry, J.T. Koehn, C.M. Glover, A. Levina, P. Lay, **D.C. Crans**

9:00 INOR 56. Synthesis, characterization, and reactivity of platinum indazole complexes with potential anti-cancer activity. **R.E. Bachman**, K. Barwick, A.J. Bachman, K.A. Wheeler

9:20 INOR 57. Mixed fluorinated subphthalocyanines and subnapthalocyanines: Tuning fluorescence by synthetic design. **K.J. McAuliffe**, L. Sejdarasi, E.R. Trivedi

9:40 INOR 58. Understanding the molecular basis of multiple mitochondrial dysfunctions syndrome 1: Impact of substitution on the structure and function of the essential iron-sulfur protein NFU1. **N. Wesley**, J. Cowan

10:00 Intermission.

10:15 INOR 59. Intramolecular hydrogen bonding between peptide strands directed by a rigid, bimetallic ring system. **T.P. Curran**, J.L. Stewart, T.T. Nguyen, J. Frempong

10:35 INOR 60. Modeling coupled binuclear copper enzymes using *de novo* designed *Due Ferri* single chain (DFsc) proteins. **B. VanDyke**, A.J. Reig

10:55 INOR 61. The IONiC/VIPEr Grand Experiment in teaching inorganic chemistry: Come join us! **B.A. Reisner**, **J.L. Stewart**

11:15 Discussion.

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S.A. Koch, *Organizer*
P.J. Farmer, Y. Zhang, *Presiding*

8:30 INOR 62. Catalysis of superoxide degradation by a Zn(II) complex with a quinol-containing ligand. M.B. Ward, M. Yu, A. Scheitler, I. Ivanovic-Burmazovic, **C.R. Goldsmith**

8:50 INOR 63. Photoswitchable probes to reversibly control the activity of carbonic anhydrase in cancer cells. **K. Aggarwal**, E.L. Que

9:10 INOR 64. Copper guanidinoquinoline complexes as entatic state models of electron transfer proteins. **J. Stanek**, A. Hoffmann, S. Herres-Pawlis

9:30 INOR 65. Tyrosinase model systems with efficient catalytic activity. **P. Liebhäuser**, C. Wilfer, A. Hoffmann, S. Herres-Pawlis

9:50 INOR 66. Multiple-site, long-distance concerted proton electron transfer in biomimetic metallopeptides. **B. Koronkiewicz**, J. Swierk, C.A. Schmuttenmaer, J.M. Mayer

10:10 Intermission.

10:20 INOR 67. A computational investigation of some mechanistic effects of metal center on regulating reactivity of heme-copper oxidase. M. Michael, Y. Shi, **Y. Zhang**

10:40 INOR 68. Mechanism-guided design of efficient P450 catalysts for C-H amination via nitrene transfer. **V. Steck**, R. Fasan

11:00 INOR 69. Quantum chemical modeling of metal-dependent decarboxylases. **F. Himo**

11:20 INOR 70. Building copper active sites in artificial metalloproteins. **S.I. Mann**, T. Heinisch, T.R. Ward, A. Borovik

11:40 INOR 71. Photo-induced oxygenations of Ru(II) bisbipyridyl flavonolate complexes. **P.J. Farmer**, X. Han, M. Kumar, M.A. Omary, M. Ghimire

12:00 INOR 72. Withdrawn.

Section J

Ernest N. Morial Convention Center
Room 212

Chemistry of Materials: Materials for Energy & Catalytic Applications

C.G. Lugmair, *Organizer*
P. Dongare, C. Schoettle, *Presiding*

8:30 INOR 73. 9,10-Dihydro-9,10-diboraanthracene salts as versatile catalysts. **E. von Grotthuss**, M. Wagner

8:50 INOR 74. (Ag)Au concave cubes as experimental models of computationally predicted active sites for the oxygen-assisted coupling of alcohols. **D. Robertson**, M.E. King, M.L. Personick

9:10 INOR 75. Highly active and stable calixarene-protected clusters for hydrogenation catalysis. **C. Schoettle**, A. Okrut, A. Palermo, A. Solovyov, A.S. Katz

9:30 INOR 76. Refinement of aerosol processes to generate highly dispersed catalytic centers for metathesis on silica supports. **B.S. Hanna**, M. Bukhovko, S.C. Hayden, S. Shaikh, M. Khokhar, S. Zhang, D.F. Consoli, Y. Roman-Leshkov, M. Ostraat

9:50 Intermission.

10:05 INOR 77. Synthesis of POSS based hybrid catalysts and their application in alkane oxidation. **A.J. Karkamkar**

10:25 INOR 78. Mechanistic investigation of alkyl benzene photooxidation by flavin photocatalyst. **P. Dongare**, I. MacKenzie, D.A. Nicewicz, T.J. Meyer

10:45 INOR 79. Characterization of and catalysis with lattice-confined reative intermediates. **D. Powers**

11:05 INOR 80. Carbonate-promoted C–H carboxylation of aromatic hydrocarbons with CO2. **D.J. Xiao**, A. Yau, M. Kanan

Section K
Ernest N. Morial Convention Center
Room 335

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
W. Lee, N.A. Piro, *Presiding*

8:30 INOR 81. From T-shaped to face-capping: A flexible bisguanidinyl pyridine ligand for Fe to Zn. J.E. Allen, **N.A. Piro**

8:50 INOR 82. Allosteric regulation of a four-state WLA macrocycle. **A. dAquino**, H. Cheng, J. Barroso, Z. Kean, J.E. Mendez, C. McGuirk, C.A. Mirkin

9:10 INOR 83. Synthesis and structural characterization of copper(I) oxalate complexes. **A.T. Royappa**, A.D. Royappa, R.F. Moral, A.L. Rheingold,

‡*Cooperative Cosponsorship*

R.J. Papoular, D.M. Blum, T.Q. Duong, **J.R. Stepherson**, O.D. Vu, B. Chen, M.R. Suchomel, J.A. Golen, G. André, N. Kourkoumelis, A.D. Mercer, A.M. Pekarek, D.C. Kelly, C.L. Stern, P. Mueller

9:30 INOR 84. Crystal structure of zirconium tetrachloride revisited. **R. Borjas Nevarez**, S.M. Balasekaran, E. Kim, P. Weck, F. Poineau

9:50 INOR 85. Electronic coupling in cationic and anionic ligand-centered, mixed-valence complexes of nickel, palladium, and platinum. **C.P. Ramirez**, A.F. Heyduk

10:10 Intermission.

10:20 INOR 86. Synthesis and characterization of an iron complex bearing a hemilabile NNN-pincer for catalytic hydrosilylation of organic carbonyl compounds. H. Lin, M. Zeller, C. Chen, **W. Lee**

10:40 INOR 87. Synthesis and structural characterizations of fluorine substituted cobalt oxo-cubes. **A. Rahman**, A. Nicolay, P. Lee, R. Lavorie, T. Tilley

11:00 INOR 88. Structural and vibrational spectroscopic studies of hexafluororhenate (IV) salts. **J. Louis-Jean**, S. Mariappan Balasekaran, D. Smith, A. Salamat, C. Pham, F. Poineau

11:20 INOR 89. Counter ion influence based on the copper(II) methylbenzoic acid complex mixed with 2,2´-bipyridine: Synthesis, X-ray characterization and biological activity. **J.A. Obaleye**, A.A. Ajibola, V.B. Bernardus

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski
Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Control of Zeolite Structure, Composition & Sites for Catalysis
Sponsored by CATL, Cosponsored by INOR

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 345

Synthetic Chemistry Addressing Challenges in Energy & the Environment
Cosponsored by CATL and WCC
L.A. Berben, A. De Bettencourt Dias, A.L. Prieto, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 INOR 90. Structural and thermochemical parameters influencing the PCET formation of a cobalt(III)-hydride. **J.L. Dempsey**, D. Kurtz, N. Elgrishi, W.C. Howland, B. Kandemir

1:55 INOR 91. Biosynthesis of the H-cluster of the [FeFe]-hydrogenase. **J.B. Broderick**

2:15 INOR 92. Surface-ligand induced stabilization of plasmonic behavior of copper sulfide nanoparticles. Z. Georgieva, M. Tomat, **K. Plass**, C. Kim

2:35 INOR 93. Aqueous chemistry of transition metal complexes of perfluoropinacolate ligands. J.E. Henebry, E.M. Laaker, **L.H. Doerrer**

2:55 Intermission.

3:00 INOR 94. Mimicking nature by metal-organic frameworks: Perspective and applications. **N.B. Shustova**, E. Dolgopolova, A.M. Rice, B. Yarbrough

3:20 INOR 95. Bio-inspired dehalogenation: Developing first-row transition metal complexes to treat priority pollutants perchloroethylene and trichloroethylene. **K.M. Van Heuvelen**

3:40 INOR 96. Manipulating the thermoelectric properties of polymer semiconductors. J. Ogle, M. Teferi, C. Boehme, **L.L. Whittaker**

4:00 INOR 97. Elemental distribution and excited state dynamics in oxynitride nanocrystals. **G. Dukovic**

Section B
Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*
B. Chen, D. Jiang, *Presiding*

1:30 INOR 98. Towardf forth generation porous coordination polymers/metal-organic frameworks. **S. Kitagawa**

2:15 INOR 99. Optimizing NIR-emitting MOFs through design and modulation of Ln-MOF platforms. **N.L. Rosi**, T. Luo, C. Liu, P. Muldoon

2:45 INOR 100. Metal-organic frameworks for programmable drug release. **H. Deng**

3:15 INOR 101. A novel application of Metal Organic Framework (MOF) as a smart fragrance delivery vehicle for consumer products. **L. Pan**

3:35 Intermission.

3:50 INOR 102. A toolkit for the modification of high valent carboxylate MOFs. **H. Zhou**, S. Yuan

4:20 INOR 103. Exchange of linkers and guests in MOFs. **A.J. Matzger**

4:50 INOR 104. Evolution of form in metal-organic frameworks. **W. Choe**

Section C
Ernest N. Morial Convention Center
Room 343

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak

J.S. Figueroa, *Organizer*
A.A. Barney, *Presiding*

1:30 INOR 105. Electrocatalytic alcohol oxidation with molecular catalysts. **R.M. Waymouth**, K.M. Waldie, E. McLoughlin, C.E. Chidsey

1:55 INOR 106. Structural and chemical aspects of metal-isocyanide network materials. **J.S. Figueroa**, D. Agnew, A. Arroyave

2:20 INOR 107. Phosphinidene chemistry stemming from anthracene-based reagents. W.J. Transue, A. Velian, M.B. Geeson, M. Nava, **C.C. Cummins**

2:45 INOR 108. Bifunctional metalloligands in MN_2S_2βRe/$Mn(CO)_3X$ complexes designed for CO_2 reduction catalysts. A.M. Lunsford, N. Arnet, S. Ding, M.B. Hall, **M.Y. Darensbourg**

3:10 Intermission.

3:30 INOR 109. Capturing intermediates of molecular catalyst/semiconductor systems by transient mid-IR spectroscopy.. **L. Hammarstrom**, M. Abdellah, M. Gilbert Gatty

3:55 INOR 110. Electrochemically-promoted catalytic asymmetric hydrogenation using chiral organorhodium complexes. **B.T. Donovan-Merkert**

4:20 INOR 111. Organometallic species at the heart of small molecule reduction catalysis. **J.C. Peters**

4:45 INOR 112. Catalytic C–H borylation: New catalysts with high regioselectivities for challenging substrates. **M.R. Smith**

Section D
Ernest N. Morial Convention Center
Room 352

ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer

C.T. Saouma, J.J. Warren, *Organizers*
S.N. Brown, *Organizer, Presiding*

1:30 INOR 113. Mechanistic studies on iron-catalyzed alkene coupling reactions. D. Kim, **P.L. Holland**, W. Rahaman, R. Poli

1:50 INOR 114. The role of amines in CO2 reduction. **C.T. Saouma**

2:10 INOR 115. Mechanistic studies of the insertion of carbon dioxide into late transition metal element sigma bonds. **N. Hazari**, J. Heimann

2:30 INOR 116. Proton relays in CO_2 reduction catalysts: Is one enough? **J.J. Warren**, S. Sinha, S. Hanson

2:50 INOR 117. Metal-oxido and metal-hydroxido complexes in biology. **A. Borovik**

3:10 Intermission.

3:20 INOR 118. Proton-electron promoted reductive O-O cleavage within synthetic heme-O_2-copper assemblies. **K.D. Karlin**, S.M. Adam, G.B. Wijeratne, P.J. Rogler, S. Sharma, I. Garcia-Bosch

3:40 INOR 119. Radical reactions at metal–oxo complexes: Revisiting old questions about metal–oxo "π radicals". **J.D. Soper**

4:00 INOR 120. Mechanisms of dinitrogen cleavage and nitride reduction to ammonia at pincer complexes. **A.J. Miller**, S. Schneider, I. Siewert, F. Hasanayn, B.M. Lindley, R.S. van Alten, Q.J. Bruch

4:20 INOR 121. Adding or removing protons and electrons in metal-mediated reduction of N_2 and oxidation of NH_3. **R. Bullock**, D. Prokopchuk, A.J. Kendall, P. Bhattacharya, E.S. Wiedner, M.T. Mock

Section E
Ernest N. Morial Convention Center
Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Roman-Leshkov, *Organizer*
Y. Surendranath, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 INOR 122. MOF-templated metallic clusters as catalysts and electrocatalysts. C. Kung, Z. Li, A. Atilgan, O. Farha, **J.T. Hupp**

2:10 INOR 123. Electrically conductive metal-organic frameworks: Insights from theory. **C.H. Hendon**

2:40 INOR 124. Metal-semiquinoid magnets: From molecules to materials. I. Jeon, J. DeGayner, L. Liu, **D. Harris**

3:10 Intermission.

3:30 INOR 125. Strategies and results for controlled activation of small-molecule zinc sensors in cells. J.M. Goldberg, **S.J. Lippard**

4:00 INOR 126. Transition metal signaling in the brain and beyond. **C.J. Chang**

4:30 INOR 127. Bioinorganic explorations of the competition for nutrient metal ions at the host/microbe interface. **E.M. Nolan**

5:00 INOR 128. Carbon-fixation pathway of the bionic leaf. C. Liu, S. Nangle, P. Silver, **D.G. Nocera**

Section F
Ernest N. Morial Convention Center
Room 354

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Cosponsored by WCC
J.S. Martinez, *Organizer*
V.L. Pecoraro, *Presiding*

‡*Cooperative Cosponsorship*

1:30 Introductory Remarks.

1:40 INOR 129. New biology revealed by tracking mobile zinc in the brain. **S.J. Lippard**

2:05 INOR 130. Metals, drugs and disease. **K.J. Franz**

2:30 INOR 131. Investigations of siderophore-mediated antibiotic delivery to Gram-negative bacteria. **E.M. Nolan**

2:55 INOR 132. Biosynthesis of methanobactin. **A.C. Rosenzweig**

3:20 Intermission.

3:40 INOR 133. In sickness and in health: Relationships between plasma metal ions and the development of infectious diseases. **P.L. Carver**

4:05 INOR 134. Seeing red: The role of heme in *Pseudomonas aeruginosa* virulence and pathogenesis. **A. Wilks**, S. Mouriño, W. Huang, A.T. Dent

4:30 INOR 135. Immunotheraphy is enhanced by vanadium compounds. **D.C. Crans**, M. Selman, J. Diallo

4:55 INOR 136. A bioinorganic-inspired approach for developing inhibitors of influenze endonuclease. **S. Cohen**, C.V. Credille, B. Dick, C. Morrison

Section G
Ernest N. Morial Convention Center
Room 210

Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/ Denitrification Reactions

K.M. Lancaster, N. Lehnert, *Organizers*
J.D. Caranto, *Presiding*

1:30 INOR 137. Bioinorganic aspects of nitrogen monoxide (NO) oxidation or reduction chemistry mediated at copper or heme centers. **K.D. Karlin**, J.J. Liu, G.B. Wijeratne, R. Cao, S. Sharma

2:00 INOR 138. A missing link from nitric oxide to nitrite in ammonia oxidizing bacteria. **K.M. Lancaster**, M. Smith, J.D. Caranto

2:30 INOR 139. Investigation of enzymatic N_2O production through isotopic analysis and engineered enzymes. **C. Finders**, E.L. Hegg, J. Haslun, N. Ostrom

2:50 INOR 140. Modeling key intermediates in Cytochrome P450 Nitric Oxide Reductase: Electronic structure and reactivity. **N. Lehnert**

3:20 Intermission.

3:30 INOR 141. A metallopeptide functional mimic of cytochrome c nitrite reductase. **K. Bren**, Y. Guo, B. Kandemir, J. Stroka

4:00 INOR 142. Probing the mechanism of microbial N_2O production. **E.L. Hegg**, C. Finders, J. Haslun, N. Ostrom, N. Lehnert

4:30 INOR 143. Influences of the heme-lysine crosslink in Cytochrome P460 over redox catalysis and nitric oxide sensitivity. **A.C. Vilbert**, K.M. Lancaster

4:50 INOR 144. Rebalancing the nitrogen cycle: Earth-abundant metal reduction of nitrate with purpose-designed ligands. **K.G. Caulton**, A. Cabelof, D.M. Beagan, J. Seo, S. braley, A.V. Polezhaev, C. Chen

Section H
Ernest N. Morial Convention Center
Room 211

Undergraduate Research at the Frontiers of Inorganic Chemistry

Catalysis, Coordination Chemistry & Materials

C. Nataro, L.A. Watson, *Organizers*
B. Fox, *Presiding*

1:30 INOR 145. Synthesis, separation, and characterization of two-dimensional tin (II) sulfide nanosheets. E. Juarez-Diaz, E.S. Aydil, **J.D. Dwyer**

1:50 INOR 146. Bio-derived building blocks for various drop in fuels and value added chemicals. **O. Staples**, C. Moore, R. Jenkins, T. Semelsberger, W. Kubic, A.D. Sutton

2:10 INOR 147. Synthesis and spectroscopic studies of rhodium pincer hydride complexes. **A. Talosig**, O. Ozerov, B. Morse, A. Larsen

2:30 Intermission.

2:45 INOR 148. Synthetic, spectroscopic, and computational study of SNS copper(I) pincer complexes based on bis-imidazole and bis-triazole precursors: Impact of ligand design and solvent coordination on conformer interconversion. **J.R. Miecznikowski**, M. Lynn, J. Jasinski, E. Reinheimer

3:05 INOR 149. High throughput synthesis of thermoelectric nanocrystals: Investigation of the lithium, zinc, antimony phase space. **K. Baumler**, A. White, A. Medina-Gonzalez, J. Vela

3:25 INOR 150. Synthesis and structural characterization of $RE_6Cd_{23}T$ (*RE* = La-Gd; *T* = late group 14, 15, or 16 element). **G.J. Desroches**, S.S. Bobev

3:45 INOR 151. Tuning cation exchange of copper chalcogenide nanoparticles. A. Unruh, B. Li, H. Le, **K. Plass**

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N.S. Radu, *Organizer*
C. Camp, J.A. Telser, *Presiding*

1:30 INOR 152. Paramagnetic resonance spectroscopy of catalytically relevant organochromium(III) complexes. **J.A. Telser**, H. Hansen, J. Krzystek, M. Enders

1:50 INOR 153. Influence of tetradentate macrocyclic ligand sterics on the conformational flexibility and photoluminescent properties of copper(I) complexes. **P. Patil**, J. Khusnutdinova

2:10 INOR 154. Synthesis, characterization and reactivity of chromium(VI) alkylidene complexes. **P. Wu**, K.H. Theopold, G.P. Yap

2:30 INOR 155. Zirconocene-amine intermolecular frustrated Lewis pairs. **H. Hamilton**, A.M. King, O. Metters, D. Wass

2:50 INOR 156. Light-dependent, zirconium-catalyzed hydrophosphination. **C. Bange**, R. Waterman

3:10 INOR 157. Towards tantalum-based early-late heterobimetallic complexes. **C. Camp**

3:30 INOR 158. Synthesis and characterisation of cyclopalladated with C^N ligand complexes for catalytic carbon hydrogen bond activation. **N.P. Yahaya**

3:50 INOR 159. Exploring Shrock cycle intermediates: Synthesis of CCC-NHC Ta bis imido complexes and their reactivity with hydrazine derivatives. **T.R. Helgert**, T.K. Hollis, C.E. Webster, J. Denny, G. Liang, B. Donnadieu

Section J
Ernest N. Morial Convention Center
Room 212

Environmental & Energy-Related Inorganic Chemistry

S.A. Koch, *Organizer*
B.L. Davis, T.M. Nenoff, *Presiding*

1:30 INOR 160. Progress toward high voltage, high cycle life non-aqueous flow cells for grid scale energy storage. T. Chu, S. Maurya, I.A. Popov, N. Mehio, E.R. Batista, P. Yang, **B.L. Davis**

1:50 INOR 161. Ligand exchange reactions of copper bipyridyl redox couples used in dye sensitized solar cells. **Y. Wang**, T. Hamann

2:10 INOR 162. Heterometallic molecular precursor for the preparation of low-temperature Li-Mn oxide. **H. Han**, A.M. Abakumov, E. Dikarev

2:30 INOR 163. N-heterocyclic carbene catalytic platforms for solar fuel conversions. **O. Luca**, A.M. Lilio

2:50 INOR 164. Capture of carbon dioxide via electrochemical concentration. **S.A. Chabolla**, J.Y. Yang

3:10 Intermission.

3:20 INOR 165. Curved carbon-rich materials for energy storage applications. **M.A. Petrukhina**

3:40 INOR 166. Structure-function trends in immobilized molecular catalysis of CO_2 reduction. **K. Prather**, J.D. Blakemore

4:00 INOR 167. Selective silica separations from waste water using ion-exchange media. **T.M. Nenoff**, K. Sasan, P.V. Brady, J. Krumhansl

4:20 INOR 168. The impact of surface chemistry and texture on the CO_2 uptake capacity of graphene oxide. **A.S. Alazmi**, O. El Tall, M. Hedhili, P. Costa

4:40 INOR 169. Stranded and shut-in gas provides a stop-gap measure for electrical demand. **S. Tedesco**

5:00 INOR 170. Nano-pyrite as a highly efficient reagent for remediation of chromate. **A.W. Apblett**, A. Bergeson, T. Reed, J. Stephens

Section K
Ernest N. Morial Convention Center
Room 335

Chemistry of Materials: Nanomaterials

C.G. Lugmair, *Organizer*
L. Wheeler, *Presiding*

1:30 INOR 171. On the use of carboxylic acid groups to graft photosensitizers on Ru nanoparticles for water splitting catalysis: Experimental and theoretical characterization of the surface composition. **R. Gonzalez Gomez**, R. Poteau, K. Philippot, C. Amiens, I. Del Rosal, L. Cusinato

1:50 INOR 172. Sequential cationic and anionic ligand exchange chemistry on cesium lead halide perovskite quantum dots for high-efficiency photovoltaics. **L. Wheeler**, A. Marshall, E. Sanehira, P. Schulz, M. Suri, N.C. Anderson, J. Berry, L. Lin, J. Luther

2:10 INOR 173. Molecular clusters as precursors for battery electrodes. **A. Pinkard**

2:30 INOR 174. Exploring the effect of nanoscale architecture on thermal conductivity of nanoporous SiO_2 films. **Y. Yan**, M. Li, S. King, J. Kang, T. Galy, Y. Hu, S.H. Tolbert

2:50 INOR 175. Low fluence multiphoton imaging with alloyed lanthanide nanocrystals. B. Tian, A. Fernandez-Bravo, E. Chan, P. Schuck, **B.E. Cohen**

3:10 INOR 176. *In vivo* X-ray imaging of transport of renal clearable gold nanoparticles in the kidneys. **J. Xu**, M. Yu, J. Zheng

3:30 Intermission.

3:45 INOR 177. PEI or GSH coated gold nanoparticles conjugated to cullin-5 DNA and heat shock protein 90 inhibitor, tanespimycin, for breast cancer therapy. **S. Talamantez-Lyburn**, E. Ehrlich, **M. Devadas**

4:05 INOR 178. Synthesis of core/ shell nanoparticles and their impact on cytotoxicity of A549 lung cells. **W.C. Corbin**, A.A. McBride, K.S. Butler, **B.A. Hernandez-Sanchez**

4:25 INOR 179. Blood biocompatible conjugate of super robust and water-soluble gold-aryl functional nanoparticles with bovine serum albumin. **A. Mohamed**, M. Karuthaka, M. Naggar, I.A. Shehadi, B. Workie

4:45 INOR 180. Manganese and iron oxo-clusters as a substitute for gadolinium in MRI contrast. **V. Dahanayake**, S.L. Stoll

5:05 INOR 181. Photo/chemo/ immunotherapy of primary tumor and remission of metastasis by using cascade upconversion nanoparticles. **J. Chen**

Actinide Complexes & Nanoclusters
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LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials

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SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

General

C. Nataro, L.A. Watson, *Organizers*

5:30–7:30

INOR 182. IONiC VIPEr: Slithering to the next stage of improving the teaching and learning of inorganic chemistry. **L.A. Watson**, **C. Nataro**, A.K. Bentley, H.J. Eppley, E.R. Jamieson, A.R. Johnson, J.R. Raker, B.A. Reisner, S.R. Smith, J.L. Stewart, N. Williams

Section B
Ernest N. Morial Convention Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic Chemistry

C. Nataro, L.A. Watson, *Organizers*

5:30–7:30

INOR 183. Synthesis of a nickel iron phosphine complex: Structural mimic of carbon monoxide dehydrogenase (CODH). **N. Sutthirat**, Z. Thammavongsy, J.Y. Yang

INOR 184. Ni^{2+} and Co^{2+} biomimetic structural analogues of the enzyme active site of acireductone dioxygenase (ARD). **A. Sanchez**, S.A. Toledo, V. Lynch

INOR 185. Investigating dechlorination abilities of bio-inspired nickel compounds. **R. Griffin-Hare**, C. Ye, B. Wada, K. Van Heuvelen

INOR 186. Cancer selective ruthenium pro-drugs have been studied to show that pH can influence the distribution coefficient and uptake. **S. Altman**, A.R. Hairston, J. Gray, F. Qu, E.T. Papish

INOR 187. Peptides linked via a methyleneamine linker to a rigid, bimetallic ring system as a possible model system for β-sheet formation. T.P. Curran, J.L. Stewart, **P.R. Handali**, **J.P. Sanderson-Brown**

INOR 188. Synthesis and conformational analysis of peptides linked to a rigid, bimetallic ring system using aromatic spacers. T.P. Curran, J.L. Stewart, L.M. Davidson, N. Pokharel, **J. Frempong**, **M.L. Phillip**, **C.B. Gober**

INOR 189. Synthesis of new tridentate ligands to model the active sites of zinc metalloproteases. **S. Bradley**

INOR 190. Altering the *de novo Due Ferri* single chain protein to mimic the structure and reactivity of coupled binuclear copper enzymes. **S. Worthington-Kirsch**, B. VanDyke, A.J. Reig

INOR 191. Exploring the electronic structure of sulfite oxidase utilizing a metal complex bearing a selenium scorpionate ligand. **S. Nichols**

INOR 192. Ru(II)-diimine complexes for cross-linking P450 enzyme aggregates. **M. Do**, **M. Kato**, **L.E. Cheruzel**

INOR 193. Investigation of $^{89}Zr^{+4}$ chelation for positron emission tomography. **A. Chung**, M. Abdalrahman, B. Barron, R.P. Planalp

Section C
Ernest N. Morial Convention Center
Hall D

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Cosponsored by WCC
J.S. Martinez, *Organizer*

5:30–7:30

INOR 194. Iron and gold nanoparticles, where do they go? Bioanalytical techniques to measure metal content by ICP-MS. **H.M. Neu**, K. Ok, S.A. Alexishin, M.A. Kane, J.E. Polli, S. Teymorian, M.H. Griep, S.L. Michel

INOR 195. Mechanistic investigations of thioesterase domain in siderophore biosynthesis. **A. Jelowicki**, Z.L. Reitz, A. Butler

INOR 196. A photoreactive marine siderophore from an *Alcanivorax* species with unique iron binding capabilities. **C.D. Hardy**, A. Butler

INOR 197. A suite of asymmetric siderophores produced by a marine *Shewanella* species. **J. Carmichael**, A. Butler

INOR 198. Genomics-based expansion of a natural combinatoric library of siderophores. **Z.L. Reitz**, K. Dulaney, A. Butler

Section D
Ernest N. Morial Convention Center
Hall D

Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/ Denitrification Reactions

K.M. Lancaster, N. Lehnert, *Organizers*

5:30–7:30

INOR 199. Synthesis and characterization of cytochrome P460 active site model complexes. **R.E. Coleman**, K.M. Lancaster

INOR 200. Withdrawn

INOR 201. Role of redox non-innocence in a Co-based nitrate reduction electrocatalyst. **G.R. Ware**, D.C. Ashley, E. Jakubikova

INOR 202. Elucidating the role of nitrosocyanin in ammonia-oxidizing bacteria. **M. Smith**, J.D. Caranto, K.M. Lancaster

INOR 203. Investigating the mechanism of cytochrome P460 from the methanotroph *Methylococcus capsulatus* (Bath). **S.H. Majer**, K.M. Lancaster

INOR 204. A mechanistic view of Cytochrome c nitrite reductase (ccNiR)-catalyzed reduction of nitrite to nitric oxide- a partial reduction of six-electron reduction of nitrite to ammonia (ammonification)- by weak reducing agent. **M. Ali**

INOR 205. New synthetic model that relevant to NO reduction by flavordiiron NO reductases. **H. Dong**, C.J. White, N. Lehnert

INOR 206. Spectroscopic analysis of *Nitrosomonas europaea* cytochrome C_{554} mutant F156H. **D.P. Koltermann**

Section E
Ernest N. Morial Convention Center
Hall D

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

D.C. Lacy , C.G. Riordan, J.Y. Yang, *Organizers*

5:30–7:30

INOR 207. Remotely operated systems for primary recovery of ^{99}Mo from accelerator-driven sub-critical fission of LEU. **J.F. Krebs**, A. Youker, J. Byrnes, K. Quigley, S. Chemerisov, G. Vandegrift

INOR 208. Coordination chemistry of organomanganese phenolic-pincer complexes. **K. Kadassery**, S.N. MacMillan, D.C. Lacy

INOR 209. Synthesis and characterization of a high-spin Fe-NO enzyme model complex with H-bond donors. **B. Burke**, M. Martin, G.P. Yap, R.C. Scarrow

INOR 210. Quantification of non-idealized hapticity in aza-heterocyclic adducts of Manganocene. **A.F. Cannella**, S. Dey, S.N. MacMillan, D.C. Lacy

INOR 211. Investigation of a peroxomanganese(III) species supported by a diazacycloalkane-based tetradentate ligand. **M. Denler**, T.A. Jackson, G.B. Wijeratne

INOR 212. Modulating the catalytic activity of first-row transition metal catalysts supported by redox-active ligands. **C.B. Kovel**, O. Villanueva, J.K. Elinburg, C.E. MacBeth

INOR 213. Nickel(II) catalyzed aziridination reactions. **D. Liu**, J. Bacsa, C.E. MacBeth

INOR 214. New (μ-Hydroxo)(μ-peroxo) diiron(III) complex: Structure, magnetism, Mössbauer spectra, and reactivity. **A. Kumar**

INOR 215. Withdrawn.

INOR 216. Ligand-based reductions in iron pyridinediimine complexes with protonated secondary coordination spheres. **P. Cheung**, J.D. Gilbertson

INOR 217. Effect of the second coordination sphere on reactivity of monomeric manganese complexes with terminal oxido and hydroxido ligands. **C. Sun**, S. Barman, J.R. Jones, A. Borovik

INOR 218. Mechanistic studies of cobalt-mediated C–H activation of aminoquinoline-directed biaryl coupling reactions. **E.E. Liu**, C.E. MacBeth, J. Bacsa

INOR 219. Biosynthetic inorganic chemistry: Artificial metalloproteins. **K.R. Miller**, S.I. Mann, D. Brazzolotto, L. Olshansky, A. Borovik

INOR 220. Biosynthetic inorganic chemistry. **V. Oswald**, J.L. Lee, C. Sun, D.L. Ross, J.A. Bogart, J.L. Kneebone, S.K. Barman, A. Borovik

INOR 221. Symmetric azulene-based π-linkers asymmetrically functionalized with isocyanide and mercapto junctions. **J. Applegate**, N.R. Erickson, N. Gerasimchuk, M.V. Barybin

INOR 222. Polyelectrochromism of diisocyanide-terminated, linear bi- and terazulenic platforms. **N.R. Erickson**, A.D. Spaeth, D.M. McGinnis, M.V. Barybin

INOR 223. Syntheses and structural comparison of $[Co(DIG_3tren)X]BPh_4$ complexes (X = halide). **D. Suryavanshi Magar**, R.C. Scarrow, G.P. Yap, M. Martin

INOR 224. Enticing anion reduction with Lewis acids in the secondary coordination sphere of iron (II) pyridinediimine complexes. **K.T. Burns**, J.D. Gilbertson

INOR 225. Exerting extreme π-acidity of isocyanoazulene ligands through cyanation of the azulenic scaffold. **Z.A. Wood**, M.D. Hart, J.J. Meyers, N. Gerasimchuk, M.V. Barybin

INOR 226. Functional diversity in gentisate 1,2 dioxygenases: A spectroscopic study. **R. Gupta**, E. Eppinger, J. Gröning, A. Stolz

Section F
Ernest N. Morial Convention Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic Chemistry, Coordination Chemistry & Catalysis

C. Nataro, L.A. Watson, *Organizers*

‡*Cooperative Cosponsorship*

5:30–7:30

INOR 227. Synthesis of dimeric zinc complexes for use as ring opening polymerization catalysts. **K.D. Brooks**, D.B. Green, A.L. Rheingold, J.M. Fritsch

INOR 228. Synthesis of chiral tridentate ligands for titanium and tantalum catalyzed asymmetric hydroamination. **A.R. Johnson**, **B.S. Mitchell**

INOR 229. Tuning hydrosilylation of hydrocarbons with substituted alpha-diimine iron(II) bromide precatalysts. **C.C. Cody**, C.E. Schulz, H.M. Hoyt

INOR 230. Synthesis of alkali and alkaline earth metal-NNN pincer complexes. **D. Haugh**, B. Wilson, A.Y. O'Brien, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

INOR 231. Catalytic ring closing reactions of gold compounds containing bis(phosphino)ferrocene ligands. **T.A. Michaels**, C. Nataro

INOR 232. Synthesis, spectroscopy properties, structural and electrochemistry characterization of two novel heterometallic pentanuclear complexes. **K. Gutierrez**, D. Pinero

INOR 233. Progress toward development of Ni/Zn phosphineoxide catecholate bimetallic olefin polymeraztion catalysts. **Y. Nguyen**, T. Tran, L. Do

INOR 234. Tris(diphenylphosphinomethyl) phenylborates with electron donating and withdrawing groups at the bridgehead boron phenyl substituent. **S. Senthil**, J.T. Stephan, M. Swift, E.T. Chan, P.J. Fischer

INOR 235. An investigation of distant inductive effects on donation into group VI metals in tris(diphenylphosphinomethyl) phenylborate complexes. **J.T. Stephan**, S. Senthil, M. Swift, E.T. Chan, M.V. Vollmer, V.G. Young, Jr., P.J. Fischer

INOR 236. Design and synthesis of polymetallic coordination compounds. **J. Tami**, J.R. Jiménez, R. Plamont, R. Lescouëzec

INOR 237. Mixed-valent copper-based electrocatalysts for the oxygen evolution reaction. **B.H. Torda**, J.K. Nagle

INOR 238. Electronic and spectroscopic properties of [Ru(tpy)(tpyph(OH))] $[PF_6]_2$ and [Ru(tpyph(OH))$_2$][PF_6]$_2$ (tpy = 2,2':6',2''-terpyridine; tpyph(OH) = 4'-(4-hydroxyphenyl)-2,2':6',2''-terpyridine). **C.L. Montgomery**, **C.N. Teahan**, S.L. Shepherd, T. Dudley, D.P. Harrison, J.J. Paul

INOR 239. Synthesis of transition-metal catalysts with diverse potential reactivity. **A.A. DeLucia**, K. Omolo, J.P. Sadighi, L.G. Habgood

INOR 240. Mechanochemical synthesis of chiral and achiral diphosphine dioxide manganese(II) complexes: Polymorphs and solid-state photoluminescence. N. Rabaey, M. Stamp, **D.E. Janzen**

INOR 241. Synthesis of heavy donor antimony ligands coordinated to 3D metals for structural and electronic studies. **S. Shubert**, L. Taylor, M.J. Rose

INOR 242. Reaction of quinolinethiols with $Fe_3(CO)_{12}$. **B. Simkhada**, C.A. Mebi

INOR 243. Iron carbonyl complexes with mercaptopyridines. J. DeArmond, S. McLendon, E. Boraj, F. Oliver, **C.A. Mebi**

INOR 244. Synthesis of copper complexes with 3-hydroxyimidazole-1-oxide as potential single molecule magnets. **C.C. Taylor**, P. Baran

INOR 245. Gold(III) complexes for intramolecular functionalization of strong, sp^3-hybridized C-H bonds. **G.R. Donalson**, **B. Probsdorfer**, K.M. Gilmore, J.E. Thompson, M. Sleck, D. Ohlson, N.A. Curry, H.R. Murphy, O.A. Rodriguez, K. Saucedo Chavez, A.L. Rheingold, D.R. Weinberg

INOR 246. CO_2 bond scission via a [P_2Si]Rh silylene intermediate. **P.O. Peterson**, T.M. Donnell, M.T. Whited

INOR 247. Acceptorless dehydrogenation of alcohols using Cp*Ir(pyridinesulfonamide)Cl complexes. **E. Schreiber**, A.R. O'Connor

INOR 248. Rare earth complexes with sulfonamidoquinoline ligands: Synthesis and applications. **S.M. Rumrill**, N. Sequeira, A. Morillo, B.C. Chan

INOR 249. Copper(II) dimer liquid crystals: Effects of axial ligation with caprolactam. **R. Katz**, B.W. Mussleman, K.A. Wheeler, T.W. Clayton

INOR 250. Synthesis of cyclopentadienyl-Co(III) *N*-heterocyclic carbene or phosphite complexes as a starting point to explore cobalt mediated C-H bond cleavage. **C.W. Frye**, J.P. Lee

INOR 251. Tosylimido transfer reactions with copper complexes of 2,6-bis(tbo) pyridine. **J.E. Allen**, N.A. Piro

INOR 252. Catalytic activity of dioxovanadium(V) salicylaldehyde semicarbazone complexes in oxidation reactions: effect of electron directing groups. **O.Q. Conover**, M.A. Bernard, G.J. Mason, V.P. McCaffrey

INOR 253. Utilizing molybdenum complexes bearing oxygen-donating scorpionate ligands as sulfite oxidase biomimetic models. **N. Fitzpatrick**

INOR 254. Metallation of [O,O,N,O] ligands obtained from amino acid precursors for applications in polymerization. **C.M. Laux**, A. Anderson-Wile

INOR 255. Water soluble phosphate Schiff-base complexes as detectors for selenate in water. **E. Gier**, L. Jefferies

INOR 256. Catalytic activity of dioxovanadium(V) salicylaldehyde semicarbazone complexes in oxidation reactions: Scope of reaction. **M.A. Bernard**, O.Q. Conover, G.J. Mason, V.P. McCaffrey

INOR 257. Computational investigation of sulfonyl fluoride activation using bidentate NHC ligands and nickel. **N.J. Chan**, M. Ogba, D.J. O'Leary, N.D. Ball

INOR 258. Synthesis and characterization of indium (III) redox active ligand complexes. **K.E. Camacho**, A. Arnold, N. Phan, L.A. Berben

INOR 259. Sensitizing lanthanide luminescence with CMPO-based ligands. **A.T. Henry**, A.K. Mulville, E.K. Connor, S.M. Biros, E.J. Werner

INOR 260. Variation of extraction conditions for selective lanthanide chelation utilizing tripodal CMPO ligands. **E.K. Connor**, A.K. Mulville, E.J. Werner, A.T. Henry, S.M. Biros

INOR 261. Photocatalytic water oxidation by dicopper-dihydroxo complex. **K. Loveridge**, P. VanNatta, M.T. Kieber-Emmons

INOR 262. Homogeneous catalysts for the conversion of epoxides to alcohols. **A.N. Rainsberry**, J.G. Sage, **M.L. Scheuermann**

INOR 263. Mechanistic investigations of reductive elimination from Pt(IV) systems. **C. Roleder**, **E. Stephens**, **E. Zepeda**, N. Williams

INOR 264. Progress towards heteroleptic alkaline earth metal silyl amides. **M. Cousins**, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

Section G
Ernest N. Morial Convention Center
Hall D

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Thomas B. Rauchfuss

Z.M. Heiden, L.F. Szczepura, *Organizers*

5:30–7:30

INOR 265. Synthesis of novel rhenium selenide clusters containing Fischer carbene ligands. **C.P. Chin**, D.N. Huh, W. Wilson, L.F. Szczepura

INOR 266. Exploring the chemistry of Re and Mo based octahedral hexanuclear clusters. **L.F. Szczepura**

INOR 267. Green syntheses using BASIL technique. **P.F. Brandt**

INOR 268. Atom-economical homogeneous catalytic reduction of CO_2 to commodity chemicals. **W. Chu**, K.I. Goldberg

INOR 269. Electrochemical H_2 oxidation enabled by metal-to-metal hydrogen atom transfer. **G. Chambers**, E.S. Wiedner, R. Bullock

INOR 270. Metallodithiolate ligands as pendant base in [Fe^IFe^I], [Fe^I[Fe(NO)]^{II}] and [(μ-H)$Fe^{II}Fe^{II}$] systems. **K. Kariyawasam Pathirana**, P. Ghosh, C. Hsieh, N. Bhuvanesh, M.Y. Darensbourg

INOR 271. Probing photochemical processes of [FeFe]-hydrogenase model compounds by combined spectroscopic/computational study. **S. Niu**, A. Nelson, P.M. De La Torre, C.F. Works, M.B. Hall

INOR 272. Synthesis of secondary phosphines by copper-catalyzed P–C cross-coupling reaction. **M. Frik**, A.L. Haber, E.B. Schiff, **J.M. Camara**

INOR 273. Synthesis and reactivity of molecular fluorescent pincer complexes. **J.L. Fernandez**, Z.M. Heiden

INOR 274. Beyond common bonding, ferrocene-transition metal interactions. **M. Ringenberg**

INOR 275. Synthesis and characterization of hydrophobic [(β^6-arene)Ru(L)Cl_2 complexes. **A.L. Eckermann**, L.A. Miller, C. Chamberlain, V. Drust, C. Davenport

Section H
Ernest N. Morial Convention Center
Hall D

ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer

S.N. Brown, C.T. Saouma, J.J. Warren, *Organizers*

5:30–7:30

INOR 276. Mapping the variable reactivity of oleate-capped cerium dioxide nanoparticles. **R. Agarwal**, D. Damatov, J.M. Mayer

INOR 277. Tuning the electronics of *p*-substituted tris(amidophenoxide) molybdenum complexes. **A.N. Erickson**, S.N. Brown

INOR 278. Exploring differences in bonding between group 10 bis(iminosemiquinone) complexes. **K. Conner**, S.N. Brown

INOR 279. Marcus inverted region in photo-induced proton coupled electron transfer. **G.A. Parada**, S. Kolmar, B. Pettersson, L. Hammarstrom, J.M. Mayer

Section I
Ernest N. Morial Convention Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Main Group Chemistry

C. Nataro, L.A. Watson, *Organizers*

5:30–7:30

INOR 280. Systematic computational studies of ene reactions between $(F_3C)_2B{=}N(CH_3)_2$ and substituted alkenes. S.E. Hammer, J.M. Lafferty, K.R. Lawson, J.R. Gustafson, A.L. Gille, **B.C. Dutmer**, T.M. Gilbert

INOR 281. Preparation of (alkylaminomethylene)indoles and their corresponding main group complexes. **N.R. Wills**, **S. Sabbagh**, N.B. Kingsley

INOR 282. Synthesis and analysis of major pentavalent thioarsenicals. **R. Rivera**, C. Fan, Y. Cai

Section J
Ernest N. Morial Convention Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Materials, MOFs & Solid-State Chemistry

C. Nataro, L.A. Watson, *Organizers*

5:30–7:30

INOR 283. Nanocasting – Introducing secondary supports into metal-organic frameworks to increase thermal stability of the nodes. **J. Duan**, C. Malonzo, S.P. Desai, T. Webber, Z. Li, O.K. Farha, J.T. Hupp, C. Lu, R. Penn, A. Stein

‡*Cooperative Cosponsorship*

INOR 284. Actinide aqueous hydrolysis reactions: Initial steps in actinide aggregation. **D. Xia**, A. Gomez, M. Vasiliu, D.A. Dixon

INOR 285. Synthesis of MOF-templated mixed-metal oxides for catalytic carbon monoxide oxidation. **J. Bence**, C.W. Abney

INOR 286. Growth kinetics and cytotoxicity effects of surface modified zinc oxide quantum dots. **J.K. Davis-Gunn**, **D.M. McCall-Butler**, D. Francis, P.P. Benz, A. Schrock, P. Cavnar, K. Molek, A. Mena, B. Colon

INOR 287. Synthesis, characterization, and catalytic activity of hollow Mn_3O_4 nanoparticles for cyclohexene oxidation. **C.M. Karki**, J.D. Hoefelmeyer

INOR 288. Decorating carbon electrodes with gold nanoparticles to study the kinetics of redox reactions. **G.E. Kamm**, T. Le, **E.M. Ness**, J.C. Lytle, J.F. Parker, D.R. Rolison, J.W. Long

INOR 289. Application of the underlying chemistry in $PbTiO_3$ for the design of new polar perovskites. **A. Kandel**, G. Laurita-Plankis

INOR 290. Immobilization of earth abundant metals coordinated in heterobimetallic ligand scaffolds on metal organic frameworks. **K. Riley**, S.P. Desai, J. Vitillo, C. Lu

INOR 291. Precursor development of iron nanopowders for nanoink Aerosol Jet 3D printing. **D. Perales**, T.J. Boyle, N.S. Bell, A.W. Cook, L.J. Treadwell, D. Reinholtz

INOR 292. Kinetic investigation into the mechanisim for H_2 activation on supported Au nanoparticles. **C. Peterson**, S. Kumar, T.N. Whittaker, C. Pursell, L. Grabow, B. Chandler

INOR 293. Host:Guest chemistry inside a series of zirconium-based metal-organic frameworks. **C. Sparrow**, G.J. McManus

INOR 294. Solving gold-containing intermetallic compounds using an automated inorganic crystal structure refinement tool. **G. Viswanathan**, A. Oliynyk, E. Antono, J. Ling, B. Meredig, J. Brgoch

INOR 295. Experimental and computational studies of anisotropic hardness in NiP_2. **A. Lim**, J. Brgoch, A. Mansouri

INOR 296. Structural and optical properties of $Ba_3Y_2B_6O_{15}:Ce^{3+}$: A cubic borate with extremely narrow, high efficiency photon emission. **S. Hariyani**, A.C. Duke, J. Brgoch

INOR 297. New transition metal and alkali metal complexes containing the hydrotris(3,5-dimethyl-1,2,4-triazolyl) borate ligand. **B.A. Reisner**, B.C. Chan, E.T. Roberts, E.C. Krist, T. Hain, A.R. Losquadro

INOR 298. Synthesis and analysis of liquid crystals based on copper (II) tetramers. **A.M. Iradukunda**, T.R. Helgren, T.W. Clayton

INOR 299. Encapsulation of fluorescent probes within the pores of a metal-organic framework. **L. Lamos**, G.J. McManus

INOR 300. Probing surface recombination at functionalized silicon(111) surfaces. **J. Speller**, D. Boucher, M.J. Rose

INOR 301. Modification of the metal coordination sites on 1D coordination polymers. **B.J. Johnson**, N. Ibrahim, W.A. Stubbs

INOR 302. Encapsulation of molecules in metal-organic frameworks. **B.J. Johnson**, **S. Smith**, **D. Moe**

INOR 303. Synthesis and characterization of liquid crystalline properties of heteroleptic copper(II) dimers using 2-propyl valerate ligands. **Y.F. Wittmer**, C. Oscar, T.W. Clayton

INOR 304. Surface chemistry of protein-capped gold nanoparticles. Z.A. Schonrock, **A.K. Bentley**

INOR 305. Synthesis and characterization of two-dimensional SnS nanoparticles. **E. Juarez Diaz**, J.D. Dwyer, E.S. Aydil

INOR 306. High room temperature separation of CO_2 vs. C_2H_2 and N_2 in Mn(II) acetylenic phosphine-based metal organic framework. **K.M. Walsh**, J. Reynolds, B. Li, B. Chen, S.M. Humphrey

INOR 307. Designing flexible ligands for the synthesis of breathable metal-organic frameworks. **N. Giorgi**, G.J. McManus

INOR 308. Cholesteric liquid crystalline porphyrin VOC sensors. **M.E. Zick**, M.R. Ramsey, J.E. Winklarek, A.L. Dorfner, J.C. Kranick, L.J. Tucker, J.L. O'Donnell

INOR 309. Synthesis and characterization of novel phosphine coordination materials (PCMs) implementing a tetrahedral phosphonium ligand with M(III) ions. **D. Kristek**, J. Reynolds, S.M. Humphrey, A. Bohnsack

INOR 310. Synthesis and structural characterization of Ba_2SrGaO_4F. R. Green, **V. Pierre**

INOR 311. Determination of inorganic water contaminants via quantum dot doped MOFs using fluorescence spectroscopy. **K. Parson**, K.T. Jackson

Section K
Ernest N. Morial Convention Center
Hall D

Main Group Chemistry

T.W. Hudnall, *Organizer*

5:30–7:30

INOR 312. Structures and rotational dynamics of (triarylmethyl)germane propellers. **M.C. Franke**, S.J. Stoudt

INOR 313. Structural studies of alkaline earth and rare metal *trans*-azobenzene complexes. A.G. Goos, D. Weissmann, J. Pichler, J. Binder, D. Allis, **S. Vonn Dyke**, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

INOR 314. Synthesis and reactivity studies of cationic diborane compounds. **H. Liu**, **W. Yen**, C. Chiu

INOR 315. Synthesis and reactivity studies of metallylenes. **T. Lin**, **I.F. Yu**, C. Chiu

INOR 316. Synthesis and characterization of functionalized organosilicate systems. **M.A. Boucher**, K.M. Specht, L.S. Dake

INOR 317. Photochemistry of main group / late transition metal complexes. **E.S. Tabei**, S. Sen, F.P. Gabbai

INOR 318. Luminescent 1*H*-1,3-benzazaphosphole derivatives. **S. Evariste**, A.L. Rheingold, C. Moore, J. Heinicke, J.D. Protasiewicz

INOR 319. Structure function analysis: The role of metal-fluorine interactions in controlling coordination chemistry in alkaline earth metal compounds. Y. Takahashi, B. Wilson, **A.Y. O'Brien**, D. Allis, M.M. Gillett-Kunnath, K. Ruhlandt-Senge

INOR 320. $H[Al(OTeF_5)_4]$ – Synthesis and application of a Brønsted superacid. **A. Wiesner**, T.W. Gries, S. Riedel

Section L
Ernest N. Morial Convention Center
Hall D

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Roman-Leshkov, Y. Surendranath, *Organizers*

5:30–7:30

INOR 321. Non-planar multidentate metallolinker in metal-organic framework: Synthesis and catalytic performance. **C. Sun**, M. Dinca

INOR 322. Lithium-ion conductivity in oligo-ethylene oxide functionalized covalent organic frameworks. **D.A. Vazquez-Molina**, G. Pope, A. Ezazi, F.J. Uribe-Romo

INOR 323. Investigation of electronic structures of two dimensional conductive metal organic frameworks. **L. Yang**, M. Dinca

INOR 324. Conductive metal-organic frameworks for gas sensing. **Y. Ge**, M. Dinca

Section M
Ernest N. Morial Convention Center
Hall D

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Dwight S. Seferos

M.R. Jones, A.M. Spokoyny, *Organizers*

5:30–7:30

INOR 325. Ring expansion as a route to unique boron heteroarenes. **S. Yruegas**, C. Martin

INOR 326. Exploring Diels-Alder chemistry of boroles. **J.J. Baker**, C. Martin

Section N
Ernest N. Morial Convention Center
Hall D

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak

J.S. Figueroa, *Organizer*
5:30–7:30

INOR 327. Ultra thin layer of iron porphyrin COFs for CO_2 reduction in water. **P.L. Cheung**, S. Lee, S. Masaoka, C.P. Kubiak

INOR 328. Covalent attachment of $[Ni(alkynyl\text{-}cyclam)]^{2+}$ catalysts to the glassy carbon electrode. **A. Zhanaidarova**, C.P. Kubiak

INOR 329. Revealing and predicting the stability of Pt^{II}-containing molecular gyroscope isomers. **A. Ehnbom**, H. Joshi, S. Kharel, L.M. Pérez, M.B. Hall, J.A. Gladysz

INOR 330. Rh(I) diisocyanide coordination polymers for electrochemical catalyst heterogenization and semiconductor material applications. **G. Lee**, C.P. Kubiak

INOR 331. Mechanistic insight of $M(N_2S_2)$ metalloligand in Re-based electro-catalysts for CO_2 reduction. S. Ding, **Y. Tong**, M.Y. Darensbourg, M.B. Hall

INOR 332. Dynamic exchange on the ultrafast timescale. **T.M. Porter**, C.P. Kubiak

INOR 333. Electron exchange between redox non-innocent bridging ligands in mixed-valent hydrogen bonded Ru_3O clusters. **G.P. Heim**, T.M. Porter, C.P. Kubiak

INOR 334. Photoelectrochemical reduction of CO_2 through the attachment of $Re(bpy)(CO)_3Cl$ derivatives to p-type Si. **C. Miller**, C.P. Kubiak

INOR 335. New synthetic routs to functionalized P_2N_2 ligands. **F.M. Brunner**, C.P. Kubiak

INOR 336. Thermodynamic insights for the development of nickel-based CO_2 reduction catalysts. **A.L. Osterichert**, C.P. Kubiak

INOR 337. Altering the electronic structure of nanoparticles through external stimuli. **L.M. Mawby**, B.J. Lear

INOR 338. Hydricity and other thermodynamic considerations for CO_2 reduction. **K.M. Waldie**, C.P. Kubiak

Section O
Ernest N. Morial Convention Center
Hall D

Electrochemistry

B.L. Lucht, *Organizer*

5:30–7:30

INOR 339. Novel confined PFSA/Pt-zeolite composite membrane for self-humidifying PEMFC. R. Deng, **J. Song**, W. Han, K. Yeung

INOR 340. Electrochemical analysis of Ru(II) complexes with redox non-innocent S_2N_2 ligands and their applications in the reduction of CO_2. **J.A. Luna**, G. Durgaprasad, K.D. Spielvogel, C. Haas, S.K. Shaw, S.R. Daly

INOR 341. Electrocatalytic methods for O-atom transfer reactions. **T.A. Stinson**, T. Donadt, C.G. Martin, O.R. Luca

INOR 342. Porous silicon composites for high-capacity metal-ion batteries. **M.L. Anger**, B.D. Fahlman

‡*Cooperative Cosponsorship*

INOR 343. Selenium redox chemistry: From surface reactivity to biological applications. **M. Diagne**, **G. Nemeth**, **E. Wiita**, M.C. Buzzeo

INOR 344. Test-bed for detecting WSNs in Labview via unmanned vehicles. **D. Burks**

INOR 345. Cyclic voltammetric studies of *Sulfobacillus thermosulfidooxidans* using a pyrite working electrode. **R. Blake**, Z. Huang, R. Painter, Z. Wang

Section P
Ernest N. Morial Convention Center
Hall D

Environmental & Energy-Related Inorganic Chemistry

S.A. Koch, *Organizer*

5:30–7:30

INOR 346. Ionic conductivities and ion dissociation in silyl nitrile electrolytes with $LiPF_6$ and LiTFSI salts for applications in lithium-ion batteries. **S. Beecher**, **T. Derrah**, L.J. Lyons

INOR 347. Testing the viability of nitroxide radicals as redox shuttles in quantum dot sensitized solar cells. **C.C. Riley**, C. Mi, R. Beaulac

INOR 348. Photosensitization behavior of supramolecular Ir(III)-carborane complex in application to photocatalytic hydrogen production: Efficient visible light-driven charge separation and mediation. **S. Kim**, Y. Cho, B. Yun, C. Kim, S. Kang, H. Son

INOR 349. Photocatalytic reduction of CO_2 to CO through a mixed hybrid system with cationic iridium(III) complexes and Re(I)-complex-anchored TiO_2 catalytic particles. **H. Cheong**, S. Kim, Y. Cho, S. Choi, C. Kim, D. Cho, C. Pac, S. Kang, H. Son

INOR 350. Development of lower-energy photosensitizer for photocatalytic CO_2 reduction: Modification of porphyrin dye in hybrid catalyst system. **S. Choi**, H. Cheong, C. Kim, C. Pac, S. Kang, H. Son

INOR 351. Understanding the natural mechanisms for chromium mobilization in groundwater. **M. Houlihan**, A. Lopez, S.E. Fendorf

INOR 352. Synthesis of group 6 carbonyl complexes containing phosphine ligands for CO_2 reduction. **N. Walker**, **B.J. Bellott**

INOR 353. New moisture harvesting material from superhydrophilic Titania nanotubes. Y. Luo, **J. Song**, K. Yeung

INOR 354. Platinum@hexaniobate nanopeapods: Sensitized composite architectures for photocatalytic hydrogen evolution under visible light irradiation. **C. Davis-Wheeler Chin**, P.R. Fontenot, R.H. Schmehl, **J.B. Wiley**

INOR 355. NMR measurements of ion and solvent transport for organosilicon nitrile electrolytes. **J. Zhu**, L.J. Lyons

INOR 356. NMR diffusion studies of LiTFSI/organosilyl electrolytes. **E. Cunningham**, L.J. Lyons

INOR 357. Activation of carbon dioxide through thiolate-bridged heterobimetallic complexes. **N. Arnet**, A.M. Lunsford, X. Yang, M.Y. Darensbourg

INOR 358. Copper-based redox shuttles supported by rigid tetradentate ligands for dye-sensitized solar cells. **J. Lee**, J.W. Jurss, L. Chen, R.R. Rodrigues, J.H. Delcamp

INOR 359. Cobalt schiff base complex using a pyridinediimne backbone for hydrogen production. **P. Hutchison**, M. Kiker, C. Tinker, W.T. Eckenhoff

INOR 360. Hydrogen production using $Mo(O)_3$(tpa) complex. **C. Tinker**, W. Eckenhoff

INOR 361. Nickel Schiff base complexes for light driven H_2 production. **M. Kiker**, A. Graves, W. Eckenhoff

INOR 362. Nickel complexes with N_2S_2 ligands for electrocatalytic and light-driven production of hydrogen. **J. Dewar**, W. Eckenhoff

INOR 363. Substituent effects on the fixation of carbon dioxide to oxalate by a binuclear copper complex. **F. Khamespanah**, F.R. Fronczek, A.W. Maverick

INOR 364. Iridium dioxide nanocrystals synthesized by molten-salt method for oxygen and hydrogen evolution reactions. **S. Mohan**, Y. Mao

INOR 365. Dose measurements of stray radiation inside the first optical enclosure of beamline 8-ID-A at the national synchrotron light source-II. **K. Kelly**, **J. Zapata**, M. Harvey

INOR 366. Effects of promoters on increasing methane hydrate formation via gas-liquid interface alteration. **P. Rangsunvigit**, A. Seangsai, K. Inking

INOR 367. Sidewalk development and research. **A. Plumber**

INOR 368. Aerobic respiration on soluble iron is expressed constitutively by *Metallosphaera sedula*. **N. Pham**, O. Griswold, R. Blake

INOR 369. Aerobic respiration on soluble iron is expressed constitutively in *Sulfobacillus thermosulfidooxidans*. **O. Griswold**, N. Pham, R. Blake

INOR 370. Synthesis and characterization of organic-inorganic conjugate dyes designed for solar energy harvesting. **R.E. Bachman**, B.C. Bierman, S. Parks

Section Q
Ernest N. Morial Convention Center
Hall D

Inorganic Catalysts

S.A. Koch, *Organizer*

5:30–7:30

INOR 371. Hollow dendritic Ag/Pt nanoparticles for enhanced methanol oxidation efficiency. N. Sui, L. Wang, Q. Bai, **W. Yu**

INOR 372. Synthesis and characterization of pentadentate ligands for the formation of binuclear complexes. **A.C. Doner**, S. Striegler

INOR 373. Mechanism of the electrocatalytic hydrogen evolution and oxidation with rhenium tris(thiolate) complexes. **H. Tang**, E.N. Brothers, M.B. Hall

INOR 374. Computational study of the N_2 activation and NβN bond cleavage by a family of group 6 dinuclear [M(II), M(II)] μ-N_2 complexes (M = Mo, W) supported by the cyclopentadienyl, amidinate (CPAM) ligand environment. **J.K. Kirkland**, L.M. Duman, L.R. Sita, K.D. Vogiatzis

INOR 375. Layered, ternary water oxidation catalyst prepared by in-layer cobalt doping, and interlayer iron-oxo cluster intercalation in Mn-O-based birnessite. **L. Mohamad**, I.G. McKendry, M. Zdilla

INOR 376. Silver (Ag) enhanced poly(3,4-ethylenedioxythiophene) (PEDOT) infused TiO_2 nanofibers for improved photocatalytic degradation of chemical pollutants. **D. Dwyer**, J. Kinsley, J. DeCoste, W.E. Bernier, W. Jones

INOR 377. Synthesis, characterization, and catalytic activities of nickel(II) monoamido-tetradentate complex: Evidence for Ni^{III}-Oxo and Ni^{IV}-Oxo species. **H. Jeong**, H. Ahn, H. So, H. Lee, C. Kim

INOR 378. Synthesis, characterization, and efficient catalytic activities of a nickel(II) porphyrin: Remarkable solvent and substrate effects on participation of multiple active oxidants. **A. Kim**, D. Zhang, M. Kim, H. Jang, P. Kim, C. Kim

INOR 379. Synthesis of microporous vanadosilicate AM-6 for shape-selective photocatalytic applications. J. Mastrandea, **M. Ismail**

INOR 380. Electrocatalytic CO_2 reduction with *cis* and *trans* conformers of a rigid dinuclear rhenium complex: Comparing the isolated monometallic and cooperative bimetallic pathways. W. Yang, **S. Sinha Roy**, W.C. Pitts, R. Nelson, F.R. Fronczek, J.W. Jurss

INOR 381. Durable and highly reactive iron-oxo catalyst for hydrocarbon C-H bond functionalization. **L. Chen**, X. Su, J.W. Jurss

INOR 382. Metallodithiolates as S-donor ligands to palladium and their function as C-C cross coupling catalysts. **Z. Martinez**, P. Ghosh, M. Quiroz, M.Y. Darensbourg

INOR 383. Computational study for the mechanism of CO_2 reduction using imidazolium-functionalized Rhenium electrocatalysts. **X. Li**, S. Sung, M. Nippe, J. Panetier

INOR 384. DFT investigation on the catalytic reduction mechanisms of N_2 to NH_3 by Fe complexes. **S. Yu**

INOR 385. Polymers from bio-derived resources: Synthesis of poly(silylether) s from Furan derivatives catalyzed by a high valent salen–Mn(N) complex. **S. Vijjamarri**

INOR 386. Development of bifunctional catalysts containing hydride-relay ligands for CO_2 hydrogenation. **N. Devi**

INOR 387. Bioinspired manganese complexes with tetradentate pyridine-appended biperidine ligands catalyze olefin epoxidation. **F. Zhu**, G. Yang, A.J. Zoll, S.A. Thompson, J. Jackson, P. Milne, E.V. Rybak-Akimova

INOR 388. Synthesis, characterization, and structure of non-heme copper(II) complexes: An efficient atom transfer catalyst. H.U. Valle, K. Riley, **D.E. Russell**, D.K. Wolgemuth, S.L. Redd, S.L. Stokes, J.P. Emerson

INOR 389. Novel 5-coordinate and 6-coordinate low-valent molybdenum(VI)-dioxo complexes exhibiting deoxydehydration activity. **R. Tran**, S.M. Kilyanek

INOR 390. Syntheses and characterization of molecular cobalt complexes with pentadentate ligands for electro- and photocatalytic hydrogen production. **P. Wang**, S. Lei, M. Sow, M. Long, R. Reddy, G. Liang, C.E. Webster, X. Zhao

INOR 391. Low valent homogeneous catalysis using metal organic frameworks. **A.M. Rabon**, M.C. Young

INOR 392. Activation of benzylic and allylic C-H Bonds catalyzed by a low-spin Co(II) complex. **A.D. Bell-Taylor**, C. Goldsmith, J.D. Gorden

INOR 393. Incorporation of molecular rectifiers into homogeneous photocatalysts. **D.J. Boston**, I. Bhowmick

INOR 394. Computational investigation of the mechanism of metal-oxo catalyzed deoxydehydration. **K.A. DeNike**, S.M. Kilyanek

INOR 395. Electrocatalytic hydrogen production by bridged butterfly [2Fe-2S] catalysts. **M.O. Talbot**, D.H. Evans, R.S. Glass, D.L. Lichtenberger

INOR 396. Investigation on the electrocatalytic water splitting performance of molten salt synthesized $La_{1-x}Sr_xCoO_3$. **S. Mohan**, Y. Mao

INOR 397. Rational design and synthesis of substituted chiral BINAM ligands to improve enantioselectivity. **S. Murru**, R. Bista, M. Kim, A. Hancock

INOR 398. Transition metal doped TiO_2/reduced graphene oxide composites for highly efficient dye adsorption. **W.R. Thalgaspitiya**, S.L. Suib

INOR 399. Mesoporous Cu Al mixed metal oxides for one pot synthesis of imines. **D. Dissanayake**, S.L. Suib

INOR 400. Mesoporous manganese oxide catalyzed heterogeneous aerobic oxidation of primary amines to nitriles. **D. Rathnayake**, S.L. Suib

INOR 401. Highly efficient photochromic mesoporous tungsten oxide hexagonal tunnels for catalytic coupling of alkenes. **T.M. Premalal**, S.L. Suib

INOR 402. Computational chemistry: Active metal catalysts for the synthesis of urea. **T. Fitzpatrick**

Section R
Ernest N. Morial Convention Center
Hall D

Inorganic Spectroscopy

‡*Cooperative Cosponsorship*

C.V. Popescu, *Organizer*

5:30–7:30

INOR 403. Sensitization of lanthanides by graphene quantum dots: an exception to Kasha-Vavilov rule? **M. McDowell**, A. Metzger, J.M. Tour, A.A. Marti

INOR 404. Photooxidation of Amyloid beta fibrils by a rhenium complex. **B. Jiang**, A.A. Marti

INOR 405. Electronic structure and bonding in 1st row hetero-bimetallic complexes probed via multi-edge X-ray absorption spectroscopy. **S. Chatterjee**, J. Moore, P. Dunn, I. Tonks, C. Lu, K.M. Lancaster

INOR 406. Bridging Ni electronic structure and reactivity: A spectroscopic and theoretical approach. **I. DiMucci**, K.M. Lancaster, M.S. Sanford

INOR 407. Speciation of zinc in the weathered MSWI bottom ash by XAFS. **H. Zhang**

INOR 408. TD DFT studies on phosphorescent cyclometaleted alkynyl and phenylplatinum(II) complexes based on tridentate C^N^N-coordinating ligands. **E. Warden**, E. Javed, L. Yumin, S. Huo

INOR 409. "Intervalence-like" charge transfer in polypyridyl ruthenium complexes of 4-dimethylaminopyridine. **S.L. Guertin**

INOR 410. Pt-Pt interactions occur in solution lead to aggregation and polymorphism of bipyridine platinum(II) complexes. **R.E. Bachman**, J.L. Zahn, M.H. Hudson

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Great Hall A

ACS Awards in Inorganic Chemistry: Plenary Session

S.A. Koch, N.S. Radu, *Organizers*
B.T. Donovan-Merkert, *Organizer, Presiding*

8:15 INOR 411. Award Address (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry Sponsored by Strem Chemicals, Inc.). Metal hydrides in nature: Hydrogenase chemistry with models and the proteins. **T.B. Rauchfuss**

8:50 INOR 412. Award Address (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator Sponsored by the Gray Award Endowment). Electronically delocalized molecules and polymers that contain selenium and tellurium. **D.S. Seferos**

9:20 INOR 413. Award Address (ACS Award in Inorganic Chemistry Sponsored by the Aldrich Chemical Company, LLC). Proton-coupled electron transfer from molecules to materials. **J.M. Mayer**

9:55 Intermission.

10:05 INOR 414. Award Address (ACS Award in Organometallic Chemistry Sponsored by The Dow Chemical Company Foundation). The organometallic chemistry of CO_2 reduction. **C.P. Kubiak**

10:35 INOR 415. Award Address (Alfred Bader Award in Bioinorganic or Bioorganic Chemistry Sponsored by the Alfred R. Bader Fund). Elements of marine bioinorganic chemistry: From microbes to mussels. **A. Butler**

11:05 INOR 416. Award Address (ACS Award in Pure Chemistry Sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation). Taking MOFs to the extreme: Water, ammonia, and halogen capture and release with azolate-based materials. **M. Dinca**

11:35 INOR 417. Award Address (F. Albert Cotton Award in Synthetic Inorganic Chemistry Sponsored by the F. Albert Cotton Endowment Fund). Molecular complexity and inorganic chemistry: Utilizing non-covalent interactions to control function. **A. Borovik**

Actinide Complexes & Nanoclusters
Sponsored by NUCL, Cosponsored by INOR

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski
Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 345

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
K. Johnson, E.J. Werner, *Presiding*

1:30 INOR 418. On the difference in luminescence properties of red emitting $La_2Zr_2O_7$:Eu^{3+} and $La_2Hf_2O_7$:Eu^{3+} nanoparticles. **S. Gupta**, J. Zuniga, Y. Mao

1:50 INOR 419. Gd-based pH-sensitive MRI contrast agents. **N.N. Paranawithana**, A.F. Martins, P. Zhao, G. Kiefer, D. Sherry

2:10 INOR 420. Lanthanide luminescence and anion binding properties of tripodal iminopyridine complexes. **E.J. Werner**, S.M. Polzin, K.H. Felix

2:30 Intermission.

2:40 INOR 421. Electrochemical studies of surface-immobilized molecular lanthanide complexes. **K.J. Johnson**, D. Lionetti, J.D. Blakemore

3:00 INOR 422. Luminescent rare-earth complexes as sensitizers of singlet oxygen. **K. Johnson**, A. De Bettencourt Dias

3:20 INOR 423. Radical-bridged dinuclear and metallacyclic trinuclear lanthanide complexes. **B.S. Dolinar**, D.I. Alexandropoulos, V. Kuduva Radhakrishnan, T. James, K.R. Dunbar

3:40 Intermission.

3:50 INOR 424. Acquisition of upconversion luminescence images exciting with LEDs: A paradigm shift in upconversion imaging. **A. Baride**, J.M. Meruga, W.M. Cross, J.J. Kellar, S. May

4:10 INOR 425. BODIPY-functionalized 1,10-phenanthroline for near-infrared emitting ytterbium (III) complex. **H. He**

4:30 INOR 426. Lanthanide and actinide thiocyanate complexes. **R. Wilson**, T.J. Carter

Section B
Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*
W. Choe, N.L. Rosi, *Presiding*

1:30 INOR 427. Switchability phenomena in metal-organic frameworks: From fundamentals to functions? **S. Kaskel**

2:15 INOR 428. Recent progress on porous metal-organic frameworks for gas separation. **B. Chen**

2:45 INOR 429. Pore space partitioning and engineering of metal-organic framework materials. **P. Feng**, X. Bu

3:15 INOR 430. Crystal engineering of hybrid ultramicroporous materials for gas separation applications. **D.G. Madden**, M.J. Zaworotko

3:35 Intermission.

3:50 INOR 431. Engineering MOF porosity and functionality for highly effective gas separation and capture. H. Wang, B. Li, **J. Li**

4:20 INOR 432. Rapid hydrogen–deuterium exchange in metal-organic frameworks. **V. Stavila**, T.C. Wang, D. Cowgill, M. Allendorf

4:50 INOR 433. Ultrahigh and selective SO_2 uptake in inorganic anion-pillared hybrid porous materials. X. Cui, **Q. Yang**, R. Krishna, H. Wu, W. Zhou, B. Chen, H. Xing

Section C
Ernest N. Morial Convention Center
Room 343

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak

J.S. Figueroa, *Organizer*
C.W. Machan, *Presiding*

1:30 INOR 434. Cooperative effects between metals in chemical transformations. **T. Tilley**

1:55 INOR 435. Bringing inorganic insight to ligand design for metallic nanoparticles. **B.J. Lear**

2:20 INOR 436. Hydricity matters: From formate oxidation to CO2 reduction. **J.Y. Yang**, C. Tsay, B. Ceballos, D.W. Cunningham, S. Ruelas, N. Idris

2:45 INOR 437. Thermodynamic hydricity as a tool for understanding transition metal hydride reactivity in water and acetonitrile. **A.J. Miller**, K.R. Brereton, T.R. Cundari, C.L. Pitman

3:10 Intermission.

3:30 INOR 438. Transition metal catalyzed hydrogenation of CO_2 and carbonyl compounds. W. Chu, Z. Culakova, **K.I. Goldberg**

3:55 INOR 439. Applications of tris[(1-isopropylbenzimidazol-2-yl)dimethylsilyl] methyl and related ligands to main group and transition metal chemistry. S. Ruccolo, M. Rauch, **G. Parkin**

4:20 INOR 440. Redox non-innocence in first row transition metal chemistry. **P.T. Wolczanski**, S.P. Heins, B. Zhang, B.P. Jacobs, D. Pokhriyal, T.R. Cundari

4:45 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 352

ACS Award in Inorganic Chemistry: Symposium in honor of James Moers Mayer

S.N. Brown, J.J. Warren, *Organizers*
C.T. Saouma, *Organizer, Presiding*

1:30 INOR 441. Reaction of an iridium(III) hydride with oxygen: experimental and computational studies of the mechanism. A.M. Wright, D. Pahls, B. Gary, T. Warner, J. Williams, S. Knapp, K. Allen, C.R. Landis, T.R. Cundari, **K.I. Goldberg**

1:50 INOR 442. Asset or achilles heel? The role of the pendent base in metal-ligand cooperative dehydrogenation catalysis. **J.M. Blacquiere**, J.M. Stubbs, B.J. Bridge, E. El-Zouki

2:10 INOR 443. Olefin trimerization and ethylene tandem conversion to linear low density polyethylene. **J.E. Bercaw**

2:30 INOR 444. Predictive model for the rates of decarboxylation of silver benzoate complexes relevant to catalytic decarboxylative coupling reactions. **J.M. Hoover**, R.A. Crovak, S. Ciccone, A.P. Honeycutt

2:50 INOR 445. Mechanistic insights into the catalytic synthesis of polyesters from biorenewable feedstocks. **W.B. Tolman**

3:10 Intermission.

3:20 INOR 446. Electrocatalytic oxygen reduction with molecular catalysts and mediators. **S.S. Stahl**

3:40 INOR 447. Multiredox chemistry with *2,2′-Bipyridine Equipped with a Disulfide/Dithiol Switch.* Synthesis, electrochemistry and complexes. **M. Cattaneo**, C.E. Schiewer, A. Schober, S. Dechert, I. Siewert, F. Meyer

4:00 INOR 448. Electron flow through multicopper oxidases. **H.B. Gray**

4:20 INOR 449. Transition metal phosphide nanoparticles: Novel (pre) catalysts for water splitting. S. Mutinda, D. Li, R. Liyanage, **S. Brock**

‡*Cooperative Cosponsorship*

4:40 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Surendranath, *Organizer*
Y. Roman-Leshkov, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 INOR 450. Synthesis of materials with emergent properties. S.M. Clarke, J.P. Walsh, A. Tamerius, R.A. Klein, **D.E. Freedman**

2:10 INOR 451. Porous molecular crystals based on fluorinated aromatics and cyclobenzoins. **O. Miljanic**

2:40 INOR 452. Redox-active tunable inorganic frameworks. **A.M. Schimpf**

3:10 INOR 453. Molecular approaches to heterogeneous electrocatalysis. **Y. Surendranath**, M. Jackson, S. Oh, C.J. Kaminsky, S. Chu

3:40 Intermission.

4:00 INOR 454. Design principles for core-shell catalysts: Transition metal carbides as ideal hosts for noble metal thin films. **Y. Roman-Leshkov**

4:30 INOR 455. Correlation of electronic structure to function: Reactivity and magnetism. **T. Betley**

5:00 INOR 456. Vibronic coherence as a mechanistic probe for ultrafast dynamics in transition metal-based chromophores.. B. Paulus, E.D. Foszcz, **J.K. McCusker**

Section F
Ernest N. Morial Convention Center
Room 354

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Cosponsored by WCC
J.S. Martinez, *Organizer*
A. Butler, *Presiding*

1:30 Introductory Remarks.

1:40 INOR 457. Strategies for photo-uncaging small molecule bioregulators. **P.C. Ford**

2:05 INOR 458. Synthesis and characterization of organometallic copper nanoclusters. **T.W. Hayton**

2:30 INOR 459. Renewable polymers and ligands derived from lignin. **M.M. Abu-Omar**, S. Zhao, A. Whelton, X. Huang

2:55 INOR 460. Indoleamine 2,3-dioxygenase, the immune response and cancer. **J.T. Groves**, M.T. Nelp, P.A. Kates

3:20 Intermission.

3:40 INOR 461. Inorganic systems and interfaces for controlling bioprocesses: Hemostasis example. **G.D. Stucky**

4:05 INOR 462. Assemblies of gold, platinum and silver nanoclusters: Photophysics and catalysis. **J.S. Martinez**

4:30 INOR 463. Engineering bioinorganic functions through metal-directed protein self-assembly. **F.A. Tezcan**, L. Churchfield, J. Rittle, L. Williamson

4:55 INOR 464. Making oxygen for space travel. **H.B. Gray**

Section G
Ernest N. Morial Convention Center
Room 210

Nitrogen Un-Fixation: Mechanisms & Models of Nitrification/ Denitrification Reactions

N. Lehnert, *Organizer*
K.M. Lancaster, *Organizer, Presiding*

1:30 INOR 465. Using biosynthetic models of nitric oxide reductase (NOR) in myoglobin to elucidate structural features responsible for NOR activity and its reaction mechanism. A. Bhagi-Damodaran, J. Reed, **Y. Lu**

2:00 INOR 466. Cytochrome c nitrite reductase (ccNiR)-catalyzed reduction of nitrite to nitric oxide by ferrocyanide: Insights into the mechanism of ccNiR-catalyzed ammonification. **A. Pacheco**

2:30 INOR 467. Nucleophilic attack at the bound NO of stable ferric nitrosyl porphyrins. E.G. Abucayon, **G.B. Richter-Addo**

2:50 INOR 468. Ruthenium homogeneous catalysts for electrocatalytic oxidation of ammonia to dinitrogen at ambient temperatures. F. Habib-Zadeh, S.L. Miller, T. Hamann, **M.R. Smith**

3:20 Intermission.

3:30 INOR 469. Advances in electrocatalytic ammonia production by cytochrome c Nitrite reductases. **S.J. Elliott**

4:00 INOR 470. Homogeneous ammonia oxidation: Mechanistic investigation and catalyst development. **G. Menard**, M. Keener, C. Hunt

4:30 INOR 471. Nitrate binding and reduction by a cobalt-based electrocatalyst: the unique properties of DIM ligand. **E. Jakubikova**

4:50 INOR 472. Mechanistic studies of denitrifying heme-nonheme nitric oxide reductases. **P. Moenne Loccoz**

Section H
Ernest N. Morial Convention Center
Room 211

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic & Coordination Chemistry

C. Nataro, L.A. Watson, *Organizers*
S. Poland, *Presiding*

1:30 INOR 473. Coinage metal complexes of new N-heterocyclic thiones and selones. **D. Rabinovich**

1:50 INOR 474. Protonation state effects on the electronic properties of $[Ru(neo)_2(4,4'bpy(OH)_2)]^{2+}$ (neo = neocuproine; 4,4'bpy$(OH)_2$ = 4,4'-dihydroxy-2,2'-bipyridine). **A.M. Arcidiacono**, E.T. Papish, T. Dudley, J.J. Paul

2:10 INOR 475. Prospects for tuning Tris(diphenylphosphinomethyl) phenylborate donation via introduction of organic and organometallic substituents at the bridgehead boron phenyl group. **P.J. Fischer**, J.T. Stephan, S. Senthil, M. Swift, E.T. Chan, M.V. Vollmer, V.G. Young, Jr.

2:30 Intermission.

2:45 INOR 476. Selective catalytic reductions using Cp* iridium catalysts in formic acid/triethylamine. **J. Steets**, A.R. O'Connor

3:05 INOR 477. Catalytic asymmetric hydroamination using chiral early metal complexes of bi- and tridentate ligands. **A.R. Johnson**, C. Abelson, B.S. Mitchell, R. Karina, F. Sha, H.S. Slocumb

3:25 INOR 478. Catalytic coupling of epoxides and dry ice under mild conditions: Working toward an undergraduate laboratory experiment. **S. Poland**, T. Downs, J.B. McLemore

3:45 INOR 479. Synthesis and reactivity of palladium compounds with κ^3-bis(phosphino)ferrocene ligands. **N.E. Wamser**, **R. Bal**, C. Nataro

4:05 Concluding Remarks.

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Organometallic Chemistry: Catalysis-Early Transition Metals

N.S. Radu, *Organizer*
D. Ess, S. Groysman, *Presiding*

1:30 INOR 480. Computational design and experimental realization of chromium catalysts with control of ethylene trimerization and tetramerization. **D. Ess**, S.M. Bischof, D. Kwon, U.J. Kilgore, J.T. Fuller, O.L. Sydora

1:50 INOR 481. Cyclopropanations via heme carbenes: Basic mechanism and effects of carbene substituent, porphyrin substituent, and protein axial ligand. Y. Wei, **Y. Zhang**

2:10 INOR 482. Dinuclear pathways for the activation of strained three-membered rings. **H. Rounds**, C. Uyeda

2:30 INOR 483. Exploring nitrene sources for the titanium-catalyzed [2+2+1] formation of pyrroles. **A. Pearce**, I. Tonks

2:50 INOR 484. Earth-abundant metal catalysts for hydrogenation, hydrofunctionalization and dehydrogenative coupling reactions. **G. Zhang**, J. Aquilina, J. Cheng

3:10 INOR 485. Oxidative amination of alkene by extreme π-loading pincer N-heterocyclic carbene Tantalum bis(imido) complex. **G. Liang**, T.K. Hollis, C.E. Webster

3:30 INOR 486. Ring-opening oxidative amination of methylenecyclopropanes with diazenes via Ti^{II}/Ti^{IV} redox catalysis. **E. Beaumier**

3:50 INOR 487. Chiral ansa-zirconocenes bearing N-azolyl and related fragments:Synthesis, structure and performance in propene polymerization. V.V. Izmer, A.Y. Lebedev, I.S. Borisov, G.P. Goryunov, D.V. Uborsky, J.M. Canich, **A.Z. Voskoboynikov**

4:10 INOR 488. Heterobimetallic homogeneous catalysts for CO oxidation. **S. Groysman**, T. Hollingsworth

4:30 INOR 489. Organolanthanides and their surface organometallic catalysis for hydroboration of esters and epoxides. **S. Patnaik**, Z. Wang, J. Manzano, I.I. Slowing, M. Pruski, A.D. Sadow

4:50 INOR 490. Influence of neodymium coordination environment in ternary catalysts $Nd(RCOO)_3–AlR_3–R_2AlCl$ on the activity in 1,3-butadiene polymerization: Titration of the active sites with a poisoning agent. **D.V. Uborsky**, V.A. Kudakina, A.Z. Voskoboynikov, H. Kloppenburg, T. Gross

Section J
Ernest N. Morial Convention Center
Room 212

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*
L.M. Berreau, T.K. Hollis, *Presiding*

1:30 INOR 491. Anion effects on Cu/O_2-mediated oxidative aliphatic carbon-carbon bond cleavage reactions. **L.M. Berreau**

1:50 INOR 492. Tetradentate polypyridine transition metal complexes as water splitting catalysts. **L.M. Lifshits**, L. Kohler, L. Wickramasinghe, R.P. Thummel

2:10 INOR 493. Fluorinated copper scaffolds for ^{19}F MR-based detection of hypoxia. **D. Xie**, E.L. Que

2:30 INOR 494. Ultrafast dynamic exchange in five-coordinate complexes of ruthenium. **T.M. Porter**, C.P. Kubiak

2:50 INOR 495. Cooperative ligand-centered reactivity in transition metal complexes with triaminoborane-bridged diphosphines: Protonation turns on borane Lewis acidity. **K. Lee**, C.M. Donahue, S.R. Daly

3:10 Intermission.

3:20 INOR 496. NHC pincer complex donor ability? PtEP (Platinum (Pt) electronic parameter): A donicity scale incorporating strictly meridional, tridentate ligands. **T.K. Hollis**, C.E. Webster, M. Zhang, E.V. Dornshuld, V. Dixet, J. Camacho-Bunquin, M. Delferro

3:40 INOR 497. Photochemical dyads and triads built on rotaxane architectures. A. Ogawa, M. Bechtold, M. Wolf, J. Wytko, K. Oohora, T. Hayashi, D. Guldi, S. Campidelli, **J. Weiss**

4:00 INOR 498. Molecular underground chemical tracers for monitoring underground fluid flows. **J.M. Sears**, T.J. Boyle, R.A. Kemp, J.A. Greathouse, R.F. Hess, L.J. Treadwell

4:20 INOR 499. First row transition metal Mabiq complexes for photocatalysis. **C. Hess**

Section K
Ernest N. Morial Convention Center
Room 335

Inorganic Catalysts

S.A. Koch, *Organizer*
J. Panetier, X. Zhao, *Presiding*

‡*Cooperative Cosponsorship*

1:30 INOR 500. Toward a mechanistic understanding of selective olefin upgrading in metal-organic framework catalysts. **R.J. Comito**, E. Metzger, M. Dinca, Z. Wu, G. Zhang, J.T. Miller

1:50 INOR 501. Computational modeling of molecular electrocatalysts featuring N-heterocyclic carbenes for carbon dioxide reduction. **J. Panetier**, X. Li, K. McCardle, X. Su, J.W. Jurss, S. Sung, M. Nippe

2:10 INOR 502. Artificial photochemical reactions by metal complexes: Cofactor regeneration and CO_2 reduction. **J. Kim**, Y. Jeon, S. Kim, T. Anjong

2:30 INOR 503. Computational characterization of a visible light sensitized tellurorhodamine catalyst for thiol oxidation. **H. Irving**

2:50 INOR 504. Theoretical analysis of C-H activation of $Cp'Ir(PPh_3)$. **X. Yang**

3:10 INOR 505. Enhanced sulfide oxidation activity via tuning site environment of Zr cluster nodes in UiO-66 MOF: A synergistic experimental and computational study. **R. Limvorapitux**, H. Chen, M. Mendonca, R. Snurr, S.T. Nguyen

3:30 Intermission.

3:45 INOR 506. Water oxidation catalysis-the rate determining step? **A. Poater**

4:05 INOR 507. Performance of density functional theory for predicting hydrogenation and dimerization of ethylene using transition metal hydride catalysts supported on zeolites. **N.K. Dandu**, S.O. Odoh

4:25 INOR 508. Evidence for the photo-activation from a $[Mo_3S_7(S_2CNR_2)_3]^+$ pre-catalyst to a Mo_3S_4 core complex as a hydrogen evolution catalyst in alkaline media. **P.R. Fontenot**, B. Shan, B. Wang, S. Simpson, A.F. Greene, L.A. Hunt, N. Hammer, C.E. Webster, J.T. Mague, R.H. Schmehl, J.P. Donahue

4:45 INOR 509. Computational studies of earth-abundant macrocycle-like electrocatalysts for CO_2 reduction. **K. McCardle**, X. Su, J.W. Jurss, J. Panetier

5:05 INOR 510. Electronic and steric effects on hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution. **X. Zhao**, P. Wang, P. Li, C. Mokry, S. Lei, M. Sow, C. Odero, G. Liang, C.E. Webster

5:25 INOR 511. Density functional theory insights into rhodium-catalyzed addition of arylboronic acids to ketones. **P. Miro**, R. Recio, I. Fernandez

5:45 INOR 512. Chromium complexes in photoredox catalysis. **M.P. Shores**, R.I. Portillo, R. Higgins, D.J. Boston, A.K. Rappe

Actinide Complexes & Nanoclusters
Sponsored by NUCL, Cosponsored by INOR

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Homogeneous Catalysis for Applied Organic Synthesis
Sponsored by CATL, Cosponsored by INOR and ORGN‡

Innovative Chemistry & Materials for Electrochemical Energy Storage
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Magnetically Recoverable Catalysts
Sponsored by CATL, Cosponsored by COLL, ENFL and INOR

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix

S.A. Koch, N.S. Radu, *Organizers*

8:00–10:00

38, 42, 53, 61, 155, 189, 194, 201-202, 205, 208, 216, 230-232, 235, 257, 271-273, 275, 286, 293, 325-326, 334-335, 342, 345-347, 357-358, 364-365, 373, 380-385, 388-390, 452. See previous listings.

574, 663, 713-717, 732-734, 742-744, 746, 751, 755-757, 790, 800, 802-803, 807, 811, 813, 816-817, 823-825, 831, 834-839, 841-844, 849-850, 856-857, 863, 867, 879, 891, 897, 904, 907-908, 939-940, 942-943, 959-962, 968-970, 988-990, 993-996, 1100, 1111, 1126, 1130, 1296, 1303, 1306, 1351, 1405, 1409, 1411. See subsequent listings.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 345

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Thomas B. Rauchfuss

L.F. Szczepura, *Organizer*
Z.M. Heiden, *Organizer, Presiding*
J. van der Vlugt, *Presiding*

8:00 Introductory Remarks.

8:05 INOR 513. How nitrosyls soften first row transition metals for hydrogenase-inspired HER electrocatalysis: Mechanistic and computational studies. S. Ding, P. Ghosh, M.B. Hall, **M.Y. Darensbourg**

8:30 INOR 514. Iron thiolate catalysts for photo- electrochemical hydrogen production. **F. Gloaguen**

8:55 INOR 515. Some aspects of electrochemical and photoelectrochemical conversion of small molecules at iron sulfur clusters, diiron dithiolate and other centres.. **C.J. Pickett**

9:20 INOR 516. H_2 evolution and uptake: From biomimetic approaches to technologically relevant materials. **V. Artero**

9:45 Intermission.

9:55 INOR 517. The mechanism of nitrogen fixation by nitrogenase. **B.M. Hoffman**

10:20 INOR 518. Organometallic chemistry in the radical SAM superfamily. **J.B. Broderick**

10:45 INOR 519. Vibrational spectroscopy of hydrogen-processing enzymes using Mössbauer photons: Why the fuss about little bumps and squiggles? **S.P. Cramer**

11:10 INOR 520. Computational modeling of NiFe-hydrogenase and its biomimetic complexes. **M.B. Hall**, H. Tang, S. Niu

11:35 INOR 521. Hydrogen-evolving molecular electrocatalysts: Interplay between experiment and theory. **S. Hammes-Schiffer**

Section B
Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*
S.M. Humphrey, N.B. Shustova, *Presiding*

8:30 INOR 522. AIM-ing for catalyst synthesis with single-atom precision. Z. Li, A. Peters, J. Liu, M. Rimoldi, I. Kim, K. Otake, A. Platero-Prats, K.W. Chapman, N. Schweitzer, D.G. Truhlar, L. Gagliardi, C.J. Cramer, A.B. Martinson, O.K. Farha, **J.T. Hupp**

9:15 INOR 523. Metal-organic framework encapsulated with Lewis pair as a new paradigm for heterogeneous catalysis. **S. Ma**, Z. Niu, W. Gunatilleke

9:45 INOR 524. Unraveling the machinery of CO_2 photoreduction and water stability in titanium metal–organic frameworks. **F.J. Uribe-Romo**

10:15 INOR 525. New catalytic applications and methods of analysis of MOFs. **S. Madrahimov**

10:35 Intermission.

10:50 INOR 526. Modeling C–H Bond activation on bimetallic two-atom Co-M oxide clusters deposited on Zr-based MOF nodes. **L. Gagliardi**

11:20 INOR 527. Design strategies to coupling chemistries in dual/multi-function MOF arrays. W.A. Maza, S. Lin, **A.J. Morris**

11:50 INOR 528. Catalysis in MOFs: The characterization challenge and opportunities. **K.W. Chapman**

Section C
Ernest N. Morial Convention Center
Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

D.C. Lacy , C.G. Riordan, J.Y. Yang, *Organizers*
C.E. MacBeth, *Presiding*

8:00 Introductory Remarks.

8:05 INOR 529. Amazing nonheme high-valent iron-oxo landscape. **L. Que**

8:30 INOR 530. Primary copper(I)-dioxygen adduct formation, stabilization and substrate oxidative reactivity. **K.D. Karlin**, D.E. Diaz Romero, D.A. Quist, M. Bhadra, R. Cao

8:55 INOR 531. Mechanism of energy transfer in high quantum yield time-resolved lanthanide complexes. **K.N. Raymond**

9:20 INOR 532. Proton-coupled electron transfer. An overview. **T.J. Meyer**, P. Dongare

9:45 INOR 533. Living with oxos. **H.B. Gray**

10:10 Intermission.

10:20 INOR 534. Enhanced electron transport via material design: Impact on electrochemistry. **E.S. Takeuchi**, K.J. Takeuchi, A.C. Marschilok

10:45 INOR 535. Structure, spectroscopy and activity studies of copper-containing *Lytic Polysaccharide Monooxygenases*. **P. Walton**, G. Davies

11:10 INOR 536. Metal ligand design: Diverging approaches. W. Keown, L. Chiang, J. Gary, E.C. Wasinger, **T.D. Stack**

11:35 INOR 537. Ligand effects on the properties of formally Cu(III) complexes. **W.B. Tolman**

Section D
Ernest N. Morial Convention Center
Room 352

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B.C. Gibb, J.L. Sessler, *Organizers*
K. Bowman-James, P. Lusby, *Presiding*

8:00 Introductory Remarks.

8:15 INOR 538. Molecular containers and logic devices based on calixpyrroles. **J.L. Sessler**

8:45 INOR 539. Molecular confinement from multiple vantage points. **K. Bowman-James**

9:15 INOR 540. Cu^{II} paddle wheel-mediated dimeric capsules based on tetra-arylextended calix[4]pyrrole ligands. **P. Ballester**

9:45 Intermission.

10:00 INOR 541. Recent developments in coordination driven self-assebmly. **P.J. Stang**

10:30 INOR 542. Supramolecular recognition enhanced by hetero radical pairing interactions. **H. Li**

11:00 INOR 543. Turning capsule catalysis inside out: Novel approaches utilizing innately-polarized Pd_2L_4 scaffolds. **P. Lusby**

11:30 INOR 544. Supramolecular assemblies based on pillar-shaped

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macrocyclic compounds "pillar[n]arenes". **T. Ogoshi**

Section E
Ernest N. Morial Convention Center
Room 353

ACS Award in Pure Chemistry: Symposium in honor of Mircea Dinca

Y. Surendranath, *Organizer*
Y. Roman-Leshkov, *Organizer, Presiding*
8:30 Introductory Remarks.

8:40 INOR 545. Recent advances in olefin metathesis by molybdenum or tungsten catalysts. **R.R. Schrock**

9:10 INOR 546. Redox switchable catalysis applied to ring opening polymerization. **P. Diaconescu**

9:40 INOR 547. Biphilic organocphosphorus catalysis. **A.T. Radosevich**

10:10 Intermission.

10:30 INOR 548. Exploring dinuclear redox chemistry with silver. **M.G. Campbell**

11:00 INOR 549. Late transition metal complexes supported by "double-pincer" tetradentate ligands. **L.M. Mirica**

11:30 INOR 550. Metaphosphates: Avenues enabled by new reagents and starting materials. K. Chakarawet, **C.C. Cummins**, M.B. Geeson, Y. Jiang, S. Shepard, J. Stauber, M. Tan, W. To, Q. Wan

12:00 Concluding Remarks.

Section F
Ernest N. Morial Convention Center
Room 354

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Dwight S. Seferos

M.R. Jones, *Organizer*
A.M. Spokoyny, *Organizer, Presiding*
C.W. Machan, *Presiding*

8:30 Introductory Remarks.

8:35 INOR 551. Frustrated Lewis pair chemistry: An avenue to synthesis and catalysis. **D.W. Stephan**

9:00 INOR 552. Investigation of new photoreactivity of organoboron compounds. **S. Wang**, K. Yuan, S. Mellerup, D. Yang

9:25 INOR 553. Resolving orbital pathways for charge transfer at the interface. **C.P. Berlinguette**, C.W. Kellett, F.G. Parlane, G.J. Meyer, W. Swords, M.D. Turlington

9:50 INOR 554. Earth-abundant molecular electrocatalysts for the reduction of CO_2 and O_2. A. Nichols, S. Chatterjee, S. Hooe, **C.W. Machan**

10:15 Intermission.

10:25 INOR 555. Light-driven redox chemistry of antimony compounds. **F.P. Gabbai**

10:50 INOR 556. Catalytic and self-assembly routes to functional molecules and materials. **I. Manners**

11:15 INOR 557. Organoboron compounds in cross coupling chemistry and as catalysts for FLP reductions. **C.M. Crudden**

11:40 INOR 558. Boron clusters as dopants for solid-state and polymer materials. **A.M. Spokoyny**

12:05 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials
Cosponsored by PHYS
J.L. Dempsey, C. Heyer, E. Leon, *Organizers*
G.J. Meyer, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 INOR 559. Proton-coupled electron transfer in artificial photosynthesis and photoreduced nanoparticles. **S. Hammes-Schiffer**

8:30 INOR 560. New synthetic methods and aqeuous electrochemical characterization of p-Type $CuGaO_2$ nanocrystals. A.R. Combs, **B.H. Farnum**

8:50 INOR 561. Surface chemistry and intercalation as strategies to tune reactivity in colloidal transition metal dichalcogenide electrocatalysts. **B.M. Cossairt**, D. Henckel, O. Lenz

9:10 INOR 562. Copper substituted TiO_2: A novel p-type anatase metal oxide and its application in dye-sensitized solar cells. **S. McCullough**, J. Cahoon

9:30 INOR 563. Photoelectrochemical performance of $BiVO_4$ photoanodes integrated with [NiFe]-layered double hydroxide water oxidation nanocatalysts. **A.M. Müller**, T.S. Sinclair, H.B. Gray

9:50 Intermission.

10:00 INOR 564. Electrochemical measurements of the redox potentials of multiply reduced colloidal semiconductor nanocrystals. C.K. Brozek, G.M. Carroll, E. Tsui, K. Hartstein, **D.R. Gamelin**

10:20 INOR 565. Nano-spectroscopy for characterization of surfaces and interfaces. **J. Atkin**

10:40 INOR 566. Fluorescence activation by visible light in conjugated polymer nanoparticles. **E.J. Harbron**, X. Zhang, H.C. Hannon

11:00 INOR 567. Design, synthesis, and passivation of metal oxide photocathodes for aqueous solution: Fixing and moving beyond NiO. **J. Cahoon**

11:20 INOR 568. Strongly coupled chromophore-base-phenol dyads: PCET oxidation on surfaces and using polymetallic chromophores. **G. Manbeck**, J.J. Concepcion, E. Fujita

11:40 INOR 569. PCET with colloidal quantum dots: Quantification of surface proton concentration and demonstrations of PCET-mediated colloidal catalysis. **E.A. Weiss**, S. Lian, D. Westmoreland, K. McClelland

Section H
Ernest N. Morial Convention Center
Room 211

Solid-State Inorganic Chemistry

C.G. Lugmair, V. Poltavets, *Organizers*
B. Saparov, *Presiding*

8:30 INOR 570. The origin of unusual valence band structure in layered bismuth oxyhalides. **H. Kageyama**

8:50 INOR 571. Hybrid Organic-Inorganic Halides of Group 12 Metals (Zn, Cd, Hg): syntheses, crystal and electronic structures, and prospective optoelectronic applications. **B. Saparov**

9:10 INOR 572. Bringing node-and-linker principle out in metal-free systems: Enlarged diamond-like networks from halogen-bonded halide ions. **C.A. Gunawardana**, M. Dakovic, C.B. Aakeroy

9:30 INOR 573. Intrinsic broadband white-light emission from ultrastable, cationic lead halide materials. Z. Zhuang, C. Peng, **H. Fei**

9:50 INOR 574. Rapid microwave synthesis of organically-grafted layered perovskites and exfoliated nanosheets. S. Akbarian-Tefaghi, A. Poduval, E. Teixeira Veiga, G. Amand, **J.B. Wiley**

10:10 Intermission.

10:25 INOR 575. Chemically controlled design and discovery of new materials. **T. Tran**, M. Quintero, K. Arpino, X. Wang, T. McQueen

10:45 INOR 576. Borides and carbaborides as transition-metal-free intercalation cathodes with redox active anions. **V. Poltavets**, M.R. Shabetai, J.Y. Do

11:05 INOR 577. Non-icosahedral high-pressure boron allotrope. **I. Chuvashova**, E. Bykova, M. Bykov, V. Prakapenka, K. Glazyrin, L. Dubrovinsky, N. Dubrovinskaia

11:25 INOR 578. Searching for new superconductors with chemistry view. **X. Gui**

11:45 INOR 579. Structurally related carbometalates grown from Pr/Ni flux. T.O. Engstrand, **S.E. Latturner**

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S.A. Koch, *Organizer*
J.L. Brumaghim, R.S. Khnayzer, *Presiding*

8:30 INOR 580. Diiridium (III) and Ru(II) complexes as emission probes for cell imaging and cellular activities. **J. Kim**, T. Anjong

8:50 INOR 581. DNA interactions of potent thione and selone antioxidants: Control via metal coordination? S. Goodman, **J.L. Brumaghim**

9:10 INOR 582. Rational design of a cytotoxic dinuclear Cu_2 complex that binds by molecular recognition at two neighboring phosphates of the DNA backbone. **T. Glaser**

9:30 INOR 583. Withdrawn

9:50 INOR 584. Development and study of novel ruthenium complexes as potential dual-activated anticancer prodrugs: The role of pH in uptake and the use of cytotoxic ligands. **J. Gray**, F. Qu, J. Park, A. Shrestha, S. Altman, A.R. Hairston, Y. Kim, E.T. Papish

10:10 Intermission.

10:20 INOR 585. Napthoquinone fused N-heterocyclic carbene-Gold(I) complexes as dual targeting cancer therapeutics. **K. Arumugam**, J. Arambula, M. Miles, R. McCall

10:40 INOR 586. Pyridine modified heterocycles and coordination complexes derived from first row transition metals. **K.N. Green**, S.M. Brewer, H.M. Johnston

11:00 INOR 587. Structure-activity relationships for a new class of Mn-based MRI contrast agents: Magnetic relaxation, protein binding, and pharmacokinetics. **E. Gale**

11:20 INOR 588. Syntheses, characterization, and biological activities of 2-(benzylimino)methyl) -6-methoxyphenol and its metal(II) complexes. **O. Adewusi**

11:40 INOR 589. Photodynamic therapy of cancer using a long-lived Cu(I) bis-phenanthroline sensitizer. C. Al Hageh, M. Al Assad, Z. El Masri, M. El Sibai, C. Khalil, **R.S. Khnayzer**

Section J
Ernest N. Morial Convention Center
Room 212

Chemistry of Materials: Nanomaterials

C.G. Lugmair, *Organizer*
M. Friedfeld, *Presiding*

8:00 INOR 590. Circular dichroism of CdSe nanocrystals bound by chiral carboxylic acids. **M. Puri**, V.E. Ferry

8:20 INOR 591. Halide-terminated cadmium selenide nanocrystals: From classic fundamental chemistry to devices. **N.C. Anderson**, J.S. Owen

8:40 INOR 592. Kinetically controlled heterostructure assembly of cadmium chalcogenide nanorods. **M. Enright**, B.M. Cossairt

9:00 INOR 593. Measurement and theoretical modelling of multiply charged quantum dot redox potentials. **C.K. Brozek**, H. Liu, X. Li, D.R. Gamelin

9:20 INOR 594. Insights in the nucleation and growth mechanism of colloidally stable indium phosphide nanomaterials. **M. Friedfeld**, B.M. Cossairt

9:40 INOR 595. Exfoliation and surface tunability in layered rhenium chalcogenide networks. **B. Choi**

10:00 Intermission.

10:15 INOR 596. Cation exchange induced evolution of InP magic-sized cluster physical and electronic structure. **J. Stein**, B.M. Cossairt

10:35 INOR 597. Nonclassical synthetic phase control at the nanoscale. **A. Ritchhart**, B.M. Cossairt

10:55 INOR 598. Aminophosphines as versatile precursors for the synthesis of group II metal phosphide nanocrystals. **M.**

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Mundy, B.M. Cossairt

11:15 INOR 599. Phase transitions in transition metal chalcogenide superatomic crystals. **E.S. O'Brien**

11:35 INOR 600. Colloidal synthesis of metal germanide nanocrystals. T. Dupper, **A. Hochbaum**

11:55 INOR 601. Frustrated quantum dots, the experimental validation of a computational model. **J.K. Bindra**, L. Gutsev, G. Strouse, N. Dalal, S. Stoian, J. van Tol

Section K
Ernest N. Morial Convention Center
Room 335

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
M. Stollenz, E.M. Villa, *Presiding*

8:30 INOR 602. Oxygen-exchange kinetics of the Anderson-type polyoxometalate ion $IMo_6O_{24}^{5-}$. **E.M. Villa**, M.R. Spriet

8:50 INOR 603. Reactivity of a μ_3-nitridotriiron cluster. **B.J. Cook**, D.M. Ermert, R. Garcia, L.J. Murray

9:10 INOR 604. Bioinspired monooxygenase mimics: Towards the design of functional high valent metal-oxo intermediates. **J. Bogart**, S.A. Cook, A. Weitz, N. Levi, C. Moore, A.L. Rheingold, M.P. Hendrich, A. Borovik

9:30 INOR 605. Divergent electronic structures and reactivity profiles in bimetallic copper imide complexes. **K.M. Carsch**, T. Betley

9:50 INOR 606. Trapped intermediate of Meerwein-Pondorf-Verley reduction of hydroxy benzaldehyde using titanium alkoxides. **T.J. Boyle**, J.M. Sears, K.A. Dunnigan, D.R. Wheeler

10:10 Intermission.

10:20 INOR 607. Highly luminescent copper^{I} bis(amidinate) clusters and digold bis(amidine) complexes. **M. Stollenz**, O. Ugarte Trejo, A. Calderón Díaz, N. Siwabut, N. Maya, N. Bhuvanesh

10:40 INOR 608. Synthesis, characterization, and reactivity of heterobimetallic Nb/Fe complexes supported by phosphinoamide ligands. **G. Culcu**, C.M. Thomas

11:00 INOR 609. Synthesis and characterization of a Co(II)-iodosylarene adduct. **E. Hill**, A. Filatov, J. Anderson

11:20 INOR 610. Spin ground state tuning of octahedral Fe_6 clusters and their incorporation into extended magnetic structures. **K. Anderton**, B. Malbrecht, T. Betley

11:40 INOR 611. Synthesis and reactivity of bio-inspired mononuclear transition metal complexes: Hydrocarbon functionalization with reactive oxygen species. **N. Botcha**, N. Singh, A. Mukherjee

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

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TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 345

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of Thomas B. Rauchfuss

Z.M. Heiden, *Organizer*
L.F. Szczepura, *Organizer, Presiding*
A.R. Fout, *Presiding*

1:30 INOR 612. Hydrogen oxidation electrocatalysis involving hydrogen atom transfer: A homolytic approach to a heterolytic reaction. **R. Bullock**, G.M. Chambers, E.S. Wiedner

1:55 INOR 613. Radical cyclizations catalyzed by $[NEt_4][CpV(CO)_3H]$. **J.R. Norton**, J. Kuo, J. Abuyuan, C. Lorenc

2:20 INOR 614. Supported organotungsten complexes for catalysis. **A.P. Sattelberger**, **R.R. Langeslay**, M. Delferro

2:45 INOR 615. Putting more chemistry into chemical vapor deposition, or how I learned to stop worrying and listen to Tom. **G.S. Girolami**, J.R. Abelson

3:10 Intermission.

3:25 INOR 616. Augmenting small molecule binding and activation with Lewis acids. **N.K. Szymczak**, J.B. Geri, J.J. Kiernicki, J.P. Shanahan

3:50 INOR 617. Synthesis and reactivity of BODIPY-containing metal complexes. **Z.M. Heiden**, B.L. Thompson, J.L. Fernandez, N.R. Treich

4:15 INOR 618. Redox-active and reactive ligands–new avenues for organometallic chemistry, selective bond activation and homogeneous catalysis. **J. van der Vlugt**

4:40 INOR 619. Exploring iron and cobalt-based metal-thiolate catalysts for organic synthesis. **W. Wang**

5:05 INOR 620. Iron-catalyzed oxyanion reduction. **A.R. Fout**, C. Ford, Y. Park, Z. Gordon, M. Drummond

Section B
Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, *Organizers*
H. Zhou, *Organizer, Presiding*
P.K. Thallapally, *Presiding*

1:30 INOR 621. Carbon dioxide capture in diamine-appended metal-organic frameworks. R. Siegelman, P.J. Milner, J. Martell, E. Kim, M.I. Gonzalez, A. Forse, T. Runcevski, J.A. Mason, T. McDonald, J.A. Reimer, **J.R. Long**

2:15 INOR 622. Metal-organic frameworks (MOFs) as a platform for energy applications. **Q. Xu**

2:45 INOR 623. Bimetallic metal-organic frameworks. **N.B. Shustova**, E. Dolgopolova, O. Ejegbavwo, A.M. Rice

3:15 INOR 624. Direct electrical readout sensors utilizing highly selective metal organic frameworks. **T.M. Nenoff**, L.J. Small

3:35 Intermission.

3:50 INOR 625. Commercialization of metal–organic frameworks and lessons learned. **O.K. Farha**, J. Arno, M. Weston, W. Morris, P. Siu

4:20 INOR 626. Strategies for the fabrication of MOF films and coatings. **B. Wang**

4:50 INOR 627. A simple strategy to immobilize enzyme in metal-organic frameworks. **W. Liu**, L. Liu, S. Lirio, C. Lin

Section C
Ernest N. Morial Convention Center
Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

D.C. Lacy , C.G. Riordan, J.Y. Yang, *Organizers*
R. Gupta, *Presiding*

1:30 INOR 628. Multiple-site concerted proton-electron transfers (MS-CPET). **J.M. Mayer**, J. Darcy, M. Ener, B. Koronkiewicz, T. Markle

1:55 INOR 629. Metal-coordinated ligand radical-driven reactivity. **R. Mukherjee**

2:20 INOR 630. Troger's base: A versatile platform for supramolecular chemistry. **D.L. Jameson**

2:45 INOR 631. Syntheses, structural and stability comparisons of $[Co(DIG_3tren)X]Y$, (X = halide or pseudohalide; Y = X or BPh_4). **R.C. Scarrow**, D. Suryavanshi Magar, B. Burke, G.P. Yap

3:10 INOR 632. Spectroscopy and DFT calculations of a flavo-diiron enzyme identify new structures and NO intermediates of the enzymatic cycle. A. Weitz, N.C. Giri, J.D. Caranto, D.M. Kurtz, E.L. Bominaar, **M.P. Hendrich**

3:35 Intermission.

3:50 INOR 633. Artificial metalloenzymes: Second coordination sphere interactions at their best. **T.R. Ward**

4:15 INOR 634. Discovery and application of 12-lipoxygenase inhibitors as anti-platelet agents. **T.R. Holman**

4:40 INOR 635. Mononuclear high-valent Fe(OH) and Mn(OH) corroles. **D.P. Goldberg**, J. Zaragoza

5:05 INOR 636. Carbon- and sulfur-bridged iron clusters of relevance to nitrogenase. S.F. McWilliams, A.L. Nagelski, D.E. DeRosha, N.A. Arnet, B.Q. Mercado, **P.L. Holland**

Section D
Ernest N. Morial Convention Center
Room 352

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B.C. Gibb, J.L. Sessler, *Organizers*
R. Custelcean, H. Li, *Presiding*

1:30 INOR 637. Crystalline sponge method for natural product chemistry. **M. Fujita**

2:00 INOR 638. Confinement of anion-water clusters in guanidine crystals. **R. Custelcean**

2:30 INOR 639. Anion protection and self-assembly inside cages formed from stacked macrocycles. **A.H. Flood**

3:00 INOR 640. Ten years of incarceration: A versatile, water-soluble cage. **D.A. Vosburg**, J. Nitschke

3:30 Intermission.

3:45 INOR 641. Molecular capsules constructed from mixed macrocycles seamed together by metal ions. **J.L. Atwood**, C. Zhang, R. Patil, K. Sikligar, G.A. Baker, P.H. Atwood, S.G. Atwood

4:15 INOR 642. *Endo*-functionalized molecular tubes. **W. Jiang**

4:45 INOR 643. Unique host properties of polyaromatic coordination capsules. **M. Yoshizawa**

5:15 INOR 644. Recognition and reactions in deep cavitands. **J. Rebek**

Section E
Ernest N. Morial Convention Center
Room 353

Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals

R.L. Brutchey, J. Vela , *Organizers*
B.C. Melot, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 INOR 645. Halide perovskites: New high performance semiconductors.

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M.G. Kanatzidis

2:20 INOR 646. Reducing the toxicity and improving the stability of two-dimensional halide perovskites. **D. Solis-Ibarra**, B. Vargas, P.I. Roman, P. Carmona-Monroy

2:40 INOR 647. Halide perovskites beyond $CH_3NH_3PbI_3$: Structural diversity and opportunities for semiconductor design. **D.B. Mitzi**

3:20 Intermission.

3:50 INOR 648. Looking beyond methylammonium lead iodide for next generation solar absorbers. **D. Scanlon**

4:30 INOR 649. Trends in the lone pair-induced local distortions in tin and lead halide perovskites: Are Sn and Pb in the center of the octahedron? **G. Laurita-Plankis**, D.H. Fabini, C. Stoumpos, M.G. Kanatzidis, R. Seshadri

4:50 INOR 650. Capturing the properties of lead-halide perovskites with new materials. A. Slavney, I. Smith, L. Leppart, J. Neaton, **H. Karunadasa**

Section F
Ernest N. Morial Convention Center
Room 354

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Dwight S. Seferos

A.M. Spokoyny, *Organizer*
M.R. Jones, *Organizer, Presiding*
T. Li, *Presiding*

1:30 Introductory Remarks.

1:35 INOR 651. Programmable metamaterials. **C.A. Mirkin**

2:00 INOR 652. Nanoparticle slurry technologies for chemical mechanical planarization. **T. Li**

2:25 INOR 653. Using nanoscale geometry to dictate molecular behavior in inorganic nanoparticle composites. **R. Macfarlane**

2:50 INOR 654. Polymers, plasmons, and patterns. **J.M. Buriak**, F. Liu, E.J. Luber, B. Olsen

3:15 Intermission.

3:25 INOR 655. Peptide platforms for constructing plasmonic chiroptical materials. **N.L. Rosi**, A. Merg, S. Punekar

3:50 INOR 656. Spherical nucleic acids for gene regulatory and immuno therapeutic applications. **D. Giljohann**

4:15 INOR 657. Wiring-up transition metals: Translating solution chemistry to nano-scale sensors. **T.M. Swager**

4:40 INOR 658. NMR characterization of metal nanoparticle formation, structure, and performance. **J. Millstone**

5:05 INOR 659. Spatial mapping of surface-mediated nanocrystal transformations. **M.R. Jones**

5:30 Concluding Remarks.

Section G
Ernest N. Morial Convention Center
Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials

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Cosponsored by PHYS
J.L. Dempsey, C. Heyer, E. Leon, G.J. Meyer, *Organizers*
T.A. White, *Presiding*

1:30 INOR 660. Proton coupled electron transfer bond cleavage of oxygen. **D.G. Nocera**, D.K. Dogutan, M. Qiu, G. Passard, C. Cosentin

1:55 INOR 661. PCET in metal organic frameworks: Toward photoinduced water oxidation. P. Celis-Salazar, S. Lin, **A.J. Morris**

2:15 INOR 662. Role of PCET in small molecule activation: Water oxidation and CO_2 reduction. Y. Xie, D.W. Shaffer, L. Wang, **J.J. Concepcion**

2:35 INOR 663. Iron polypyridyl complexes immobilized on metal oxide semiconductors for photocatalytic hydrogen generation. **W. McNamara**

2:55 INOR 664. New Ru complexes demonstrate ligand-centered reactivity for the reduction of CO_2. **M.R. Norris**, M. Gu, L. Paul

3:15 Intermission.

3:30 INOR 665. Increasing rates and lowering overpotentials in $[Ni(P_2^RN_2^R)_2]^{2+}$ electrocatalysts for production of H_2. **R. Bullock**, C.M. Klug, A.J. Cardenas, M.J. O'Hagan, E.S. Wiedner

3:50 INOR 666. Unlocking redox reactivity through Installation of proton relays in the secondary coordination sphere. **J.Y. Yang**, J. Kotyk, R. Combs

4:10 INOR 667. Mechanistic studies on a family of carbene-supported ruthenium complexes for electrochemical CO_2 reduction. **S. Gonell**, M.D. Massey, I.P. Moseley, C.K. Schauer, J.T. Muckerman, A.J. Miller

4:30 INOR 668. Fast detection method for analyzing CO_2 electroreduction products to probe catalyst degradation mechanism. F. Zhang, **A. Co**

4:50 INOR 669. Evaluating the potential of nanocapsules to synthetically modulate the second coordination sphere of fuel forming catalysts. **N. Elgrishi**

5:10 INOR 670. Electrocatalysis and photo-electrocatalysis of the oxygen reduction reaction. **J.M. Mayer**, M.L. Pegis, C. Wise, D. Martin, O. Jung, B. Koronkiewicz, S. Raugei, N. Kumar, J. Peper

Section H
Ernest N. Morial Convention Center
Room 211

Chemistry of Materials: Synthesis & Properties

C.G. Lugmair, *Organizer*
Y. Rao, *Presiding*

1:30 INOR 671. Chemical vapor transport synthesis of $Mn_xZn_{(1-x)}Cr_2O_4$ single crystals in a closed *ampoule* reactor: A virtual equilibrium (steady-state) model that predicts composition (x) of the deposited crystalline solid solution. **Y. Rao**

1:50 INOR 672. Low-valent coordination networks with *m*-terphenyl isocyanides based linkers. **A. Arroyave**

2:10 INOR 673. Thermolysis of heterobimetallic single-source precursors: A springboard to the synthesis of binary intermetallic compounds. **C.L. Daniels**, S. Sahu, F.P. Gabbai, J. Vela

2:30 INOR 674. Hybrid platinum (IV) iodides: progression from perovskite to hydrogen bonded frameworks. **H. Evans**, D.H. Fabini, M. Preefer, R. Seshadri, F. Wudl

2:50 Intermission.

3:05 INOR 675. Kinetic control of one-pot core/shell nanoparticles and nanoplatelets using thio- and selenoureas. **L. Hamachi**, I. Jen-La Plante, M.P. Campos, K. Qian, G. Cleveland, I. Rreza, H. Yang, E. Chan, W. Walravens, Z. Hens, A. Kuntzmann, S. Ithurria, B. Dubertret, J.S. Owen

3:25 INOR 676. Controlled speciation of transition metal ions in cadmium thiophenolate-based molecular clusters. **K.R. Kittilstved**, F. Kato

3:45 INOR 677. Molten salt synthetic method for making complex metal oxide nanoparticles. **Y. Mao**

4:05 INOR 678. Facile and controllable synthesis of Janus two-dimensional transition metal dichalcogenide monolayers. **J. Zhang**, J. Lou

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*
E.V. Rybak-Akimova, K.D. Vogiatzis, *Presiding*

1:30 INOR 679. Pyridine azamacrocycles with appended functional groups: redox reactivity and catalysis. **E.V. Rybak-Akimova**, S.G. McKenzie, T. Palluccio, H. Seidel

1:50 INOR 680. Copper guanidine quinoline complexes as catalysts in ATRP: Prediction of activities via DFT and isodesmic reactions. **T. Rösener**, A. Hoffmann, S. Herres-Pawlis

2:10 INOR 681. Ruthenium(II) polypyridyl complexes with hydroxypyridine mixed ligands: Synthesis, characterization and *in vitro* cell cytotoxicity. **J.A. Obaleye**, A.O. Rajee, A.A. Ajibola, H.F. Babamale, M.O. Bamigboye, P.O. Obaleye

2:30 INOR 682. Withdrawn.

2:50 INOR 683. Tuning the hydricity of nickel hydrides for the electrocatalytic reduction of CO_2. **A.L. Osterichер**, C.P. Kubiak

3:10 Intermission.

3:20 INOR 684. Understanding the electronic effects that control the non-heme Fe(IV)-oxo reaction channels for C-H activation. **K.D. Vogiatzis**

3:40 INOR 685. Triiron clusters containing single atom bridging ligands for dinitrogen fixation. **R.B. Ferreira**, L.J. Murray

4:00 INOR 686. Mn(IV) complexes for biochemically activated MRI contrast. **H. Wang**, P. Caravan, T. Storr, E. Gale

4:20 INOR 687. Computational modelling of the ligand tuning effect over the transition temperature in spin-crossover systems using density functional methods. **J. Cirera Fernandez**

Section J
Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Catalysis-Late Transition Metals

N.S. Radu, *Organizer*
T. Atesin, O. Ozerov, *Presiding*

1:30 INOR 688. Computational study of the mechanism of dehydrogenative borylation of terminal alkynes by SiNN iridium complexes. **O. Ozerov**, J. Zhou, C. Lee

1:50 INOR 689. Mechanistic observations of cross coupling reactions with PNP Cobalt. **B.J. Foley**, C. Palit, O. Ozerov

2:10 INOR 690. Preferential electrochemical reduction of CO_2 to formate by a CCC-NHC-Ni complex: A computational/mechanistic study. **R.W. Lamb**, J. Cope, N. Liyanage, P.J. Kelly, J. Denny, J.H. Delcamp, T.K. Hollis, C.E. Webster

2:30 INOR 691. Electrocatalytic formate oxidation with an iridium hydride complex. **K.M. Waldie**, C.P. Kubiak

2:50 INOR 692. Bioorthogonal transfer hydrogenation mediated by small molecule organoiridium catalysts. **S. Bose**, **L. Do**

3:10 INOR 693. Understanding the thermodynamic and kinetic factors that contribute to transfer hydrogenation efficiency by organoiridium complexes. **A.H. Ngo**

3:30 INOR 694. Palladium(0)-catalyzed intramolecular allylic alkylation of diketoesters. **T. Atesin**

3:50 INOR 695. Enhancing catalytic performance of phosphine-phosphinate and phosphine-phosphonate Pd alkyl polymerization catalysts by remote binding of $B(C_6F_5)_3$. **A. Johnson**, N.D. Contrella, J. Sampson, M. Zheng, R.F. Jordan

4:10 INOR 696. Carbon dioxide reduction by anionic chalcogenide-bridged tricopper clusters. **B.J. Cook**, L.J. Murray

4:30 INOR 697. Controlled $4e^-$ reduction of CO_2 with various hydroboranes and first row metal hydride catalysts. **S. Bontemps**

4:50 INOR 698. Substrate directed, enantioselective Heck arylation of cyclohexenols promoted by $KCTf_3$: Synthesis of all cis substituted, arylcyclohexenols. **R.A. Angnes**, L.M. Thompson, C.R. Correia, G.B. Hammond

5:10 INOR 699. Metal–ligand bifunctional catalysis: The "accepted" mechanism, the issue of concertedness, and the function of the ligand in catalytic cycles involving hydrogen atoms. **P.A. Dub**

5:30 INOR 700. Olefin hydroarylation catalyzed by ruthenium(II) complexes: Changes in reactivity based on auxiliary

ligands. **X. Jia**, J. Gary, B.A. McKeown, T.R. Cundari, P.J. Perez, T.B. Gunnoe

Section K
Ernest N. Morial Convention Center
Room 335

Inorganic Spectroscopy

C.V. Popescu, *Organizer, Presiding*
1:30 Introductory Remarks.

1:35 INOR 701. To be or not to be: Bonding studies in heterobimetallic d^{10}-d^{10} centers. **K. Melancon**, B.M. Otten, M.A. Omary

1:55 INOR 702. Multimodal micro-spectroscopies for metal complexes bio-imaging: development metal-CO as multimodal probes. **C. Policar**, F. Lambert, N. Delsuc, H.C. Bertrand

2:15 INOR 703. Near-field optical microscopy and nanoscale spectroscopy (nano-FTIR) on semiconductors, plasmonic and 2D materials. **P. Schäfer**, T. Gokus

2:35 INOR 704. Time-resolved IR studies in conventional and supercritical fluids: From alkane complexes and C-H activation to organometallic noble gas complexes. **M.W. George**

2:55 INOR 705. Effects of electron transfer on hydrogen bonds. **T.M. Porter**, G.P. Heim, C.P. Kubiak

3:15 Intermission.

3:20 INOR 706. Determination of the dramatic increase in protonation rates following one-electron reduction for a series of luminescent osmium hydride complexes. **R.E. Adams**, T.A. Grusenmeyer, A.L. Griffith, R.H. Schmehl

3:40 INOR 707. Theoretical study of substituted CCC-NHC palladium and platinum complexes for OLED applications. **V. Dixit**, E.V. Dornshuld, C.E. Webster, T.K. Hollis

4:00 INOR 708. Solid-state ^{45}Sc NMR of Cp^*_2Sc–R: Evidence for an agostic interaction in Cp^*_2Sc–Et. **M.P. Conley**, D. Culver, W. Huynh, H. Tafazolian

4:20 INOR 709. Direct identification of inner-sphere nitrogen radicals via nitrogen K-edge X-ray absorption spectroscopy. **J.T. Lukens**, D. Iovan, T. Kurogi, D.J. Mindiola, T. Betley, K.M. Lancaster

4:40 INOR 710. Magnetic resonance investigation of bonding between first row transition metals. **S.M. Greer**, J. McKay, K.M. Gramigna, C.M. Thomas, S. Stoian, S. Hill

5:00 INOR 711. Highly concentrated alkali hydroxide aqueous solutions: Classical force fields, speciation and their effects on neutron PDFs. **D. Semrouni**, H. Wang, K. Page, D. Wesolowski, A.G. Stack, A.E. Clark

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

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TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

Metal-Organic Frameworks: What Are Next?

W. Lin, S. Ma, H. Zhou, *Organizers*

5:30–7:30

INOR 712. Hierarchical pore formation in a series of ultrastable multivariate metal-organic frameworks. **L. Feng**, S. Yuan, L. Zhang, J. Li, A. Kirchon, H. Zhou

INOR 713. Computational modeling of the degradation of MOF-2 by Brønsted acid gases. **Z. Lee**, S. Zhang, L. Flores, **D.A. Dixon**

INOR 714. Rational design and synthesis of heterometallic metal-organic frameworks. **P. Muldoon**, C. Liu, C. Miller, N.L. Rosi

INOR 715. Arsenic coordination materials: Design, properties, and applications. **R.E. Sikma**, S.G. Dunning, P. Kunal, J. Reynolds, J. Chang, S.M. Humphrey

INOR 716. Metal-organic framework templated formation of nanostructured conducting polymers. **T. Wang**, S.K. Smoukov, A.K. Cheetham

INOR 717. Enhancing polymer crystallinity in mixed matrix membranes using metal organic framework nanosheets for efficient CO_2 capture. **C. Youdong**, D. Zhao

INOR 718. Phosphine coordination materials as a platform for catalytic metal incorporation. **S. Dunning**, G. Nandra, A.D. Conn, K.M. Walsh, W. Chai, P. Kunal, J. Reynolds, J. Chang, A. Steiner, G.A. Henkelman, S.M. Humphrey

INOR 719. Design and synthesis of multifunctional materials comprising stratified metal-organic frameworks and plasmonic nanoparticles. **T. Luo**, X. Gan, J. Millstone, N.L. Rosi

INOR 720. Ligand removal and porosity control in gradient metal-organic frameworks. **C. Liu**, Z.M. Schulte, T. Luo, N.L. Rosi

INOR 721. Chemical modifications to tailor magneto-structural correlations in the triangulated Kagome lattice $Cu_3X_2(cpa)_6$. **S.F. Skinner**, W.M. Farmer, L.W. Ter Haar

INOR 722. Aggregation to the best: A 12-connected Zirconium MOF with a triphenylene-based hexatopic linker. **Y. Zhang**, X. Yang, S. Yuan, J. Qin, H. Zhou

INOR 723. Ultramicroporous Zr MOF for C2 hydrocarbon separation. **Y. Wang**, D. Zhao

INOR 724. Preparation of 2D MOF materials. Z. Li, **K. He**, K. Yeung

INOR 725. Crystallization of sub-100 nanometer MOF thin film on graphene oxides. W. Chen, **K. He**, K. Yeung

INOR 726. MOF membrane microreactor for organic synthesis. **K. He**, K. Yeung

INOR 727. Rational design of a mixed-linker MOF platform based on merged net principle. **H. Jiang**, J. Jia, A. Shkurenko, Z. Chen, K. Adil, Y. Belmabkhout, L. Weselinski, A. Assen, D. Xue, M. O'Keeffe, M. Eddaoudi

INOR 728. Effects of chloride concentration on graphene analogues for thermoelectric devices. **S. Yoon**, M.C. So

INOR 729. Single-crystal electrical devices of triphenylene-based 2D MOFs. **R.W. Day**, M. Dinca

INOR 730. Fabrication and characterization of conductive metal-organic framework coatings by automated liquid phase epitaxy for electronics. **M.C. So**, V. Cherrette, V. Stavila, J. Llinas, A.A. Talin, M. Allendorf

INOR 731. Ultra-small face-centered cubic Ru nanoparticles confined with an anionic porous coordination cage for high performance catalysis. **Z. Xiao**, Y. Fang, H. Zhou

INOR 732. Towards the design and synthesis of metal-organic frameworks for targeted separation of heavy pollutants. **D. Fairchild**, J. Cordova, G.S. Pour, O.A. Tarano, K. Sanchez, Z. Magnuson, F.J. Uribe-Romo

INOR 733. Amenable and accessible functionality in covalent organic frameworks: Merits in the design of heavy metal scavenger for environmental remediation. **Q. Sun**, S. Ma

INOR 734. Installing biomimetic diiron complex in metal-organic framework for photocatalytic hydrogen evolution. **B.L. Frey**, X. Zhang, J. Zhang

INOR 735. One-pot synthesis of a series of zirconium MOFs with multifunctionalities. **Y. Sun**, H. Zhou

INOR 736. Cooperative enhanced catalysis of lipase-proline@MOF towards enantiomeric chemical transformation. **C. Lin**, S. Lirio, L. Liu, W. Liu

INOR 737. Porous layer network in indium based metal-organic frameworks with carbon dioxide adsorption and fixation. **C. Tsai**, Y. Li, S. Wang, C. Lin

INOR 738. Dual-ligand luminescent metal-organic frameworks towards environmental remediation efforts. **N.D. Rudd**, H. Wang, E.M. Fuentes-Fernandez, S.J. Teat, F. Chen, G.S. Hall, Y.J. Chabal, J. Li

INOR 739. Biomimetics of carbonic anhydrase via metal-organic frameworks. **Y. Chen**, Z. Zhang

INOR 740. Selective CO_2 adsorption on Cu-pyrazolato MOFs. **K. Shi**, L. Mathivathanan, R.G. Raptis

INOR 741. Fluorescent studies of melal-organic frameworks with higly conjugated linkers. **R. Ly**, G.S. Pour, F.J. Uribe-Romo

INOR 742. Titanium based metal-organic frameworks for visible light photocatalytic reduction of CO_2. **M.W. Logan**, N.V. Aleger, S. Ayad, J.D. Adamson, K. Hanson, F.J. Uribe-Romo

INOR 743. Fabricating turn on fluorescent sensors for cyanide in MOFs by sequential linker installation. **J. Li**, S. Yuan, H. Zhou

Section B
Ernest N. Morial Convention Center
Hall D

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B.C. Gibb, J.L. Sessler, *Organizers*

5:30–7:30

INOR 744. Getting specific about non-specific interactions: Functional group dependence for the inverse Hofmeister series. **J.H. Jordan**, W. Yao, A. Wishard, B.C. Gibb

INOR 745. Behavior of water under confinement in a metal-organic nanotube. **M. Payne**, A.S. Jayasinghe, T. Forbes

INOR 746. Anion specific effect on protein aggregation and precipitation. **W. Yao**, B.C. Gibb

INOR 747. Withdrawn

INOR 748. Supramolecular assemblies as a mechanistic probe: Formation and catalysis of a Si_4L_6 host. **M. Morimoto**, C.M. Hong, E.A. Kapustin, K.N. Raymond, D. Toste, R.G. Bergman

INOR 749. Supramolecular confinement of anions, from small to large, with molecular pincers. **S. Pramanik**, M. Reinmuth, H. Haque, S. Kaur, K. Motley, V. Day, K. Bowman-James

INOR 750. Molecular face-rotating cube with emergent chiral and fluorescence properties. **H. Qu**, Y. Wang, Z. Li, X. Wang, H. Fang, Z. Tian, X. Cao

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INOR 751. Larger assemblies and guest exchange in molecular containers. **A. Wishard**, L. Avram, B.C. Gibb, A. Bar-Shir

INOR 752. Does charge matter? Formation of highly reactive metal nanocluster crystal within coordination cage container. **Y. Fang**, H. Zhou

INOR 753. Designing functional supramolecules for biological applications. **I.A. Riddell**

INOR 754. Anion recognition using water-soluble hosts. **M.R. Sullivan**, W. Yao, P. Sokkalingam, B.C. Gibb

INOR 755. Electrochemical analysis of supramolecular cages as nanocapsules for catalysts. **A. Webb**, J. Bruna, S.C. Lutfallah, N. Elgrishi

INOR 756. Improving biocompatibility of nano-scale metal-organic supercontainers (MOSCs) for functional applications. **P. Jampani**, Z. Wang

INOR 757. Salt induced switching of capsular assemblies mirrors the Hofmeister effect. **M.B. Hillyer**, H. Gan, B.C. Gibb

Section C
Ernest N. Morial Convention Center
Hall D

PCET PhotoCatalysis with Inorganic Molecules & Materials
Cosponsored by PHYS
J.L. Dempsey, C. Heyer, E. Leon, G.J. Meyer, *Organizers*

5:30–7:30

INOR 758. Homogenous hydrogen evolution system employing non-noble metal bipyridyldiamine co-catalysts. **T. Vagvala**, T. Ooyabe, V. Kalousek, K. Ikeue

INOR 759. Proton transfer and proton-coupled electron transfer reactions of heteroleptic ruthenium(II) complexes incorporating hydroxylated polypyridyl ligands. **K. Martinez**, M. Esposito, E. Milner, J.J. Paul, R.H. Schmehl

INOR 760. Use of 3D ordered macroporous cuprous oxide intercalated with MoS_2 for efficient hydrogen-evolving reaction. **D.T. Conroy**, R.A. Farrer

Section D
Ernest N. Morial Convention Center
Hall D

Solid-State Inorganic Chemistry

C.G. Lugmair, V. Poltavets, *Organizers*

5:30–7:30

INOR 761. Probing formation mechanisms of templated vanadium selenites using reaction informatics. **Y. Huang**, A.J. Norquist, J. Schrier

INOR 762. The role of organic structure on phase stability in templated vanadium tellurites. **X. Jia**, A.J. Norquist, J. Schrier

INOR 763. Superhard tungsten tetraboride (WB_4): Effects of variable boron concentration and the dodecaboride forming metals on its properties. **G. Akopov**, I. Roh, Z. Sobell, M.T. Yeung, L. Pangilinan, C.L. Turner, S.I. Khan, R.B. Kaner

INOR 764. Topochemical synthesis and characterization of transition metal-fluoride double-layered perovskites, $(MF)LnNb_2O_7$ (M = Mn, Fe, Cu; Ln = La, Pr). **P. Maji**, M. Granier, D. Montasserasadi, J.B. Wiley

INOR 765. Hydrothermal synthesis and characterization of manganese doped hematite hollow spheres. **S.A. Seraly**, A.M. Morey

INOR 766. Surface functionalization and thin film deposition of β-Fe_2O_3 hollow spheres. **G.M. Harber**, J. Kittle, A.M. Morey

INOR 767. Synthesis of TMD's by chemical transformations of ultra-thin oxides: Effect of water (and chalcogen source) on morphology and the optical properties. **T. Kuykendall**, S. Aloni, A. Schwartzberg, C. Chen, C. Kastl

INOR 768. Promoted hydride/oxide exchange reaction in $SrTiO_3$ by introduction of anion vacancy. **F. Takeiri**, T. Yamamoto, Y. Kobayashi, H. Kageyama

INOR 769. Facile synthesis of metal sulfide based chevrel phases. **J. Ortiz Rodriguez**, J. Perryman, J.M. Velázquez

INOR 770. Synergy in properties and chemistry: Development of PbS QDs embedded in Pb-halide perovskite matrices. **E.A. Gaulding**, J. Luther

INOR 771. New transparent conductors. **M.T. Yeung**, S.M. Flynn, A.E. Wustrow, J.C. Hancock, K.R. Poeppelmeier

INOR 772. Understanding distortions in the cubic pyrochlore lattice towards the design of polar materials. **S. Husremovic**, G. Laurita-Plankis, J. Li, A. Sleight, R.T. Macaluso, M. Subramanian

INOR 773. Accelerating the discovery of inorganic phosphors with the assistance of machine learning. **Y. Zhuo**, J. Brgoch

INOR 774. Energy-efficient, microwave-assisted solid-state synthesis of phase-pure ternary Ti2S4 thiospinels with applications in heterogeneous catalysis. **J. Perryman**, J.M. Velázquez

INOR 775. Honeycomb network of Au-Au bonding in intermetallic, RE-Au-Sn (RE = La, Ce, Pr, Nd) ternary phase space. **S. Lotfi**, J. Brgoch, A. Oliynyk

INOR 776. $(1,2,6\text{-Trimethylpyridinium})_2Cu_2Br_6$: The vicinal trimethylpyridinium cation pair as supramolecular dication. **M.R. Bond**

INOR 777. Solid state variable temperature and pressure ^1H NMR analysis of templated carbon with substitutional doping. **B. Nakamoto**, C.M. Jensen

INOR 778. Crystal packing of quasiracemic mixtures of oxidiazanones. **S. Huffman**, G. Ferrence

INOR 779. Borides and carbaborides based intercalation cathodes with redox active anions. **M.R. Shabetai**, **J.Y. Do**, V. Poltavets

INOR 780. Substitution effects of metal and metalloid elements at the silicon sites of $TiMnSi_2$ compounds. **D. Matetich**, J. Allred

INOR 781. Physical property measurements for single crystal $V_{1-x}Mo_xO_2$. **M.A. Davenport**, J. Jones, J. Allred

Section E
Ernest N. Morial Convention Center
Hall D

Nanoscience

B.G. Trewyn, *Organizer*

5:30–7:30

INOR 782. Metal-enhanced fluorescence Hg^{2+} biosensor. N. Sui, L. Wang, **W. Yu**

INOR 783. Improved antimicrobial properties of copper and ascorbic acid based nanoparticle systems: Advanced drugs for a post-antibiotic era. **T.M. Dassanayake Mudiyanselage**, V. Serapiglia, K.M. Greskovich, S. Huang

INOR 784. Effect of the aggregation events on the optical properties of molecular-like gold clusters. **M. Sugiuchi**, K. Konishi

INOR 785. Gram scale surface functionalization of nanodiamond. **M.E. Taylor**, J. Bandy, A. Mensch, R.J. Hamers

INOR 786. Synthesis and spectroscopic measurements of yttrium (III) oxide nanomaterials doped with europium (III) cations. W. Wang, **A. Rahman**, P. Zhu

INOR 787. Growth kinetics and cytotoxicity effects of surface modified zinc oxide quantum dots at room and cold temperatures using CsOH and NaOH. **D. Francis**, D.M. McCall-Butler, J.K. Davis-Gunn, A. Mena, B. Colon, P.P. Benz, A. Schrock, P. Cavnar, K.S. Molek

INOR 788. Probing the electronic structure of small metallic nanoparticles using conduction electron spin resonance. **S. Cruz**, A. Silakov, B.J. Lear

INOR 789. Polyarylboranes: Nanoscale materials with interesting photophysical properties. **T. Wang**, **M.W. Lee**

INOR 790. Effects of perchlorate anions on the fabrication of surface enhanced Raman spectroscopy (SERS) sensors. **W. Mihalyi-Koch** , F. Dawood

INOR 791. Ceria–Zirconia nanoparticles as an enhanced multi-antioxidant for sepsis treatment. **M. Soh**, T. Hyeon

INOR 792. Sweat-based glucose monitoring and feedback transdermal drug delivery for diabetes treatment. **C. Song**, T. Hyeon

INOR 793. Multifunctional nanoparticle as tissue adhesive for image-guided procedures. **K. Shin**, **G. Ko**, T. Hyeon

INOR 794. Nano-mechanical and physical investigations of novel oxide nanocomposites using atomic force microscopy. **T.T. Brown**, S. Akbarian-Tefaghi, A. Blanco, Z.L. Highland, N. Kuruppu Arachchige, A.M. Taylor, J.C. Garno, J.B. Wiley

INOR 795. Metal oxide support for control over electronic properties in catalytic noble metal particles. **J. Fagan**, B.J. Lear

INOR 796. Crystalline-to-amorphous phase transition of large area $Mo_2O_2(\mu\text{-}S)_2(Et_2dtc)_2$ nanosheets. **M. Zhukovskyi**, M.K. Kuno

INOR 797. Microwave synthesis of nanocomposites via the capture of preformed nanoparticles within scrolled nanosheets. **A. Blanco**, T. Rostamzadeh, J.B. Wiley

INOR 798. Growth of gold and palladium nanoparticles inside and outside of halloysite nanotubes. **M. Islam Khan**, T. Rostamzadeh, J.B. Wiley

INOR 799. Synthesis and characterization of ZnO nanoparticles and their use as a photocatalyst. **J.D. Harris**, C.C. Pena, A.E. Harris, J. Cowan

INOR 800. Comparative toxicity of ZnO nanoparticles synthesized using different amines. **C.C. Pena**, K. Cornell, J. Cowan, J.D. Harris

INOR 801. Elucidating the mechanism of aluminum nanocrystal formation using EPR spectroscopy. **B.D. Clark**

INOR 802. Role of gold oxidation state in the synthesis of Au-$CsPbX_3$ heterostructured nanoparticles. **D. Dacres**, B. Roman, M.T. Sheldon

INOR 803. Nanostructured iron oxide electrodes for the water splitting reaction. **K. Koster**, L. Bradley, P. Kharel, F. Dawood

INOR 804. NiO nanoparticle synthesis, characterization, and toxicology. **P.T. Gwin**, C.C. Pena, K. Cornell, J. Cowan, J.D. Harris

INOR 805. Influence of particle size and stoichiometry on the magneto-electronic properties of $La_{1-x}Sr_xCoO_3$ nanoparticles. **H.A. De Santiago**, S. Mohan, M. Manno, E. McCalla, C. Leighton, Y. Mao

INOR 806. Polarization properties of semiconductor nanorods. **A. Francis**

INOR 807. Monitoring the growth of silver dendrites for large-area surface enhanced Raman spectroscopy (SERS) sensors. **A. Oh**, **N. DeBuono**, F. Dawood

INOR 808. High pressure exfoliation of layered materials. **W.H. Mak**, M.D. Kowal, E.P. Nguyen, R. Rizvi, R.B. Kaner

INOR 809. Multicolor emitting $La_2Zr_2O_7$ nanoparticles and its tunability on europium doping. **S. Gupta**, J. Zuniga, **Y. Mao**

INOR 810. Attachment of molecular catalysts to nanocrystal surfaces facilitated by anionic bridging ligands. M.R. Buck, **R.P. Murphy**

INOR 811. Development of a trimodal contrast agent for acoustic and magnetic particle imaging of stem cells. **J. Lemaster**, T. Kim, F. Chen, J.V. Jokerst

INOR 812. Characterization of electrical properties of GaAs nanowires and planar heterostructures by Kelvin probe force microscopy. **G. Matheson**, L. Geelhaar, M. Heilmann, J. Herranz

INOR 813. Translation of transition-metal based catalysis for selective sensing. **V. Schroeder**, T.M. Swager

INOR 814. Can nanotechnology help cell research for major diseases. **M. Breaux**

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Section F
Ernest N. Morial Convention Center
Hall D

Chemistry of Materials

C.G. Lugmair, *Organizer*

5:30–7:30

INOR 815. Electrochemical etching of Ti_2CT_x MXene in dilute HCl solution. **W. Sun**, M.J. Green, M. Radovic

INOR 816. Stabilizing CuPd nanoparticles via CuPd coupling to $WO_{2.72}$ nanorods in electrochemical oxidation of formic acid. **Z. Xi**, S. Sun

INOR 817. Atomically Thin Pt Coated over Intermetallic FePt Nanoparticles for Efficient Oxygen Reduction Catalysis in Fuel Cells. **J. Li**, S. Sun

INOR 818. Imaging boron nitride nanotubes (BNNTs) by single molecule fluorescence microscopy. **A. Smith**, Z. Tang, C. de los Reyes, D.M. Marincel, M. Pasquali, A.A. Martí

INOR 819. In situ ligand stripping and etching of indium phosphide nanocrystals. **R. Siramdas**

INOR 820. Room temperature, mild condition post-synthesis etching of InP nanocrystals. **M. Yazdanparast**, E. McLaurin

INOR 821. Photophysical Studies of Isomeric *N*-Heterocyclic Carbene Ir(III) Complexes and Their Applications to Deep-Blue Phosphorescent Organic Light-Emitting Diodes (OLEDs). **B. Yun**, S. Kim, J. Kim, C. Kim, S. Kang, H. Son

INOR 822. Detailed evaluation of nonradiative processes in heteroleptic cyclometalated iridium(III) complexes. **J. Kim**, S. Kim, Y. Cho, D. Cho, S. Kang, H. Son

INOR 823. Optical properties of stellated metal nanocrystals grown from seeds with planar defects. **J.D. Smith**, K.M. Koczkur, J.A. Burkhart, S.E. Skrabalak

INOR 824. Chemical decoration of boron nitride nanotubes with aliphatic carbon chains. **C.A. de los Reyes**, K.L. Walz-Mitra, A. Smith, A. Loredo, F. Frankovsky, A.A. Martí

INOR 825. Synthesis of colloidal ZnO nanoparticles and their assembly onto thin films. **R. Gaudet**, S. Ganguly

INOR 826. Computational and experimental development of heterobimetallic single source precursors to Ge-Sn heterostructures. **H. Andaraarachchi**, M.A. White, J. Vela

INOR 827. Preparation and characterization of a new organic-inorganic hybrid material with synergistically combined properties. **A.J. Rodriguez**, R.G. Raptis

INOR 828. Studies of bulk ammonia borane – polyethylene oxide hydrogen storage materials. **K. Kharel**, R. Fu, O. Gunaydin-Sen

INOR 829. New synthetic methods for generating carbon-based materials with well-controlled electronic properties: From superatomic solids to graphene nanoribbons. **I.M. Klein**, E. O'Brien, M. Paley, A. Crowther, X. Roy

INOR 830. Divalent iron atom coordination in two-dimensional microporous graphitic carbon nitride. **Y. Oh**

INOR 831. Large-scale synthesis of ultrathin lanthanide carbonate hydroxides nanowires for potential biomedical applications. **X. Zhang**, Y. Li, J. Ge, L. Qin, Y. Zheng, B. Lei, Y. Du, Z. Zheng

INOR 832. Synthesis of magnetic $CuCr_2S_4$ chalcospinel nanoparticles using single-source precursors. **F. Akbari Afkhami**, A. Gupta

INOR 833. Visible light sensitization of ferritin proteins by gold nanoparticles. **A. Bruefach**, E.B. Cerkez, K.G. Dutton, Y. Ghidey, M. Kukulka, A.M. Valentine, D.R. Strongin

INOR 834. Self-assembly of PS-*b*-PEO films as a shadow mask for GaAs nanowire deposition. **L.R. Steiner**, **S.C. Hall**, A. Christy, J.D. Harris

INOR 835. Synthesis of inorganic-organic perovskite hybrid materials via a microwave assisted method. **A. Poduval**, J.B. Wiley, S. Akbarian-Tefaghi

INOR 836. Flux growth of binary and ternary metal boride single crystals as catalysts for the hydrogen evolution reaction. **L. Alameda**, R.E. Schaak

INOR 837. Molten state synthesis of Pr^{3+} activated lanthanum hafnate nanoparticles as potential downconversion phosphor. **J. Zuniga**, S. Gupta, M. Pokhrel, Y. Mao

INOR 838. Grafted covalent organic frameworks for fast ionic conductivity. **G. Pope**, D.A. Vazquez-Molina, A. Ezazi, F.J. Uribe-Romo

INOR 839. Molecular additives for TiO_2 modification: A case study of dye-sensitized solar cells. **H. Cheema**

INOR 840. Assessing effects of varying metal carboxylate coverages on lead sulfide nanocrystal properties. **I. Rreza**, J.S. Owen

INOR 841. Cation exchange as a synthetic entryway to complex nanomaterials. **B.C. Steimle**, J.L. Fenton, R.E. Schaak

INOR 842. Ligand removal from indium phosphide nanocrystals. **S. Lee**, E.J. McLaurin

INOR 843. In-situ synthesis of LaOF phases from LaF_3 and exploration for upconversion luminescence. Y. Mao, **A. Perez**, S. Gupta, M. Pokhrel

INOR 844. Enhanced energy product of iron carbide nanorods induced by ruthenium. **B. Williams**, M. Tsui, E.E. Carpenter

INOR 845. Rationally designed plasmonic nanostructures for biosensing. **W. Qian**, Q. Su

INOR 846. Withdrawn.

INOR 847. Surface properties of WO_3/ZnO catalysts and their catalytic performance in the direct carbonylation of glycerol with CO_2 to glycerol carbonate. **L. Jiaxiong**, D. He

Section G
Ernest N. Morial Convention Center
Hall D

Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals

R.L. Brutchey, B.C. Melot, J. Vela , *Organizers*

5:30–7:30 INOR 848. Persistent dopants and phase segregation in organolead mixed-halide perovskites. **B. Rosales**, L. Men, S. Cady, M.P. Hanrahan, A.J. Rossini, J. Vela

INOR 849. Single crystal growth and characterization of R-M-X compounds ($R = CH_3NH_3$, $C_6H_5C_2H_4NH_3$, $C_6(CH_3)_5CH_2N(CH_3)_3$; M = Zn, Cd, Hg; X = Cl, Br, I). **R. Roccanova**, B. Saparov

INOR 850. Inherent directional order of methylammonium cations in lead-iodide perovskite.. **M. Zdilla**, Y. Rao, B.B. Wayland, X. Li, A. Pender, S. Ding

Section H
Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: Applications to Materials & Polymer Science

N.S. Radu, *Organizer*

5:30–7:30

INOR 851. Methodologies of extending π-conjugation in ferrocene. **D. Daigle**, J. Bergeron, U. Pokharel

INOR 852. Development of imino and amino pyridine iron(II) catalysts for atom transfer radical polymerization (ATRP). **V. Shastri**, L.M. Thierer, S.E. Jenny, M. Donley, L.M. Round, N.A. Piro, W.S. Kassel, C.L. Brown, T. Dudley, D.L. Zubris

INOR 853. Design and synthesis of Ru precursors for photoassisted chemical vapor deposition. **O.M. Hawkins**, C.R. Brewer, B. Salazar, A.V. Walker, L. McElwee-White

Section I
Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: Applications to Organic Transformations

N.S. Radu, *Organizer*

5:30–7:30

INOR 854. Dearomatization and reactivity of benzene and electron-deficient arenes promoted by π-basic transition metal complexes. **J. Smith**, J.T. Myers, K. Wilson, W. Harman

INOR 855. Multiple transition metal catalysts for mild hydrocarboxylation of alkenes with CO_2. **J.A. Rogers**, B.V. Popp

Section J
Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: Catalysis

N.S. Radu, *Organizer*

5:30–7:30

INOR 856. C-H bond activation and silylation of pyridine with diruthenium complexes. **R.M. Chin**, N. Jocic, J. Prybil, N. McClendon

INOR 857. δ–Heterocyclic carbene titanium(IV) and zirconium(IV) catalysts for the copolymerization of Cyclohexene Oxide with CO_2 . **L. Ralte**, K. Törnroos, E. Le Roux

INOR 858. Utilizing TiII/IV redox catalysis for the synthesis of unsymmetrical carbodiimides. **A. Pancoast**, E. Beaumier, I. Tonks

INOR 859. Influlence of hydrogen bonding in photocatalytic systems. **P.L. Cheung**, C.P. Kubiak

INOR 860. Withdrawn

INOR 861. Nickel-mediated fluorocarbene metathesis. **J. Guan**, M.B. Hall

INOR 862. Enantioenrichment of a molybdenum dearomatization agent by redox catalysis. **S. Dakermanji**, K. Welch, W. Harman

INOR 863. Hydrogenation of CO_2: A rational approach to catalyst design. **K. Grubel**, A.M. Appel, J.C. Linehan

INOR 864. Ester hydrogenation catalyzed by CNN-pincer and CC-bidentate complexes of ruthenium. **L.N. Le**, **J. Liu**, **T. He**, A.R. Chianese

INOR 865. A mechanistic DFT study of selective aldehyde hydrogenation by an octahedral PONOP iron catalyst. **B.S. Omar**, **F. Hasanayn**

INOR 866. Incorporation of NADH-like hydride relays into metal-phosphine catalysts for CO2 hydrogenation. **C. Zall**

INOR 867. Base-free transfer hydrogenation of alkenones with organometallic complexes bearing a triazenide ligand functionalized with pyrazole. **L. Medrano Castillo**, M. Parra-Hake, V. Miranda-Soto, M. Collazo-Flores, D.B. Grotjahn, D. Chávez, A.L. Rheingold

INOR 868. Operando infrared spectroscopic studies of iron-catalyzed hydromagnesiation of vinyl arenes. **J.A. Rogers**, B.V. Popp

Section K
Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: New Ligand Platforms

N.S. Radu, *Organizer*

5:30–7:30

INOR 869. Investigations into small molecule activation with a severely sterically crowded trigonal bipyramidal metal complex featuring a multidentate tris(phosphaalkene)phosphine ligand. **P. Miura-Akagi**, M.L. Nakashige, M. Cain, A.L. Rheingold

INOR 870. Derivatized mixed-ring heterocyclic and antenna carotene ligands. V. KomReddy, **D. Rillema**, H. Nguyen, A.J. Cruz, C. Moore, N.K. Senaratne, L. Kadel, D.M. Eichhorn

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INOR 871. Acid-modulation of scorpionate ligands for modern organometallic chemistry. **P. Shivokevich**, A. Heyer, W. Harman

INOR 872. Synthesis and coordination chemistry of a new PNP pincer featuring phosphaalkene and pyrrolide type-donors. **M.M. Riek**, M. Cain, A.L. Rheingold

INOR 873. Efficient synthesis of imidoylamidines. **C.R. Guifarro**, E.V. Rybak-Akimova

INOR 874. Synthesis and coordination of a new tris N-heterocyclic carbene. **M. Montgomery**, **S. Allison**, **A. Duenas**, N. Harris, D. Tapu

INOR 875. Development of new bis N-heterocyclic carbene: Synthesis and coordination chemistry. **A. Mason**, **M.A. Baker**, A. Carter, **D. Tapu**

INOR 876. New cerberus-type N-heterocyclic carbenes: Synthesis and coordination. **R. Hooper**, **J. Malone**, D. Tapu

INOR 877. Toward the synthesis and characterization of a new NHC-palladium complex. **N. Harris**, G. Crimmins, G. Bettler, A. Changas, D. Tapu

INOR 878. Synthesis and reactivity of pincer ligands containing mixed phosphine/stibine donors. **A.J. Kosanovich**, A.M. Jordan, O. Ozerov

INOR 879. Synthesis and reactivity of polydentate 1,3,5-triazine based ligands. **S. Gunther**, O. Ozerov

Section L
Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N.S. Radu, *Organizer*

5:30–7:30

INOR 880. Synthesis of Ti imidos with varying covalent donor ligands and their application in Ti redox catalysis. **T.A. Wheeler**, I. Tonks

INOR 881. Reduction of titanium imidazolin-2-iminato complexes for the activation and cleavage of N_2. **M.A. Baeza**, R. Aguilar, A. Metta-Magana, S. Fortier

INOR 882. Low-valent early transition metal CCC-NHC pincer complexes. **V. Adiraju**, C.E. Webster, T.K. Hollis

INOR 883. Reactivity study of a masked "Ti(II)" complex. **A. Jordan**, R. Aguilar, S. Fortier

INOR 884. Withdrawn

Section M
Ernest N. Morial Convention Center
Hall D

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N.S. Radu, *Organizer*

5:30–7:30

INOR 885. Synthetic methodologies for organometallic polyacenes. **J.T. Bergeron**, D. Daigle, U. Pokharel

INOR 886. Formic acid dehydrogenation: Ruthenium does it better. **N. Anderson**, A.M. Tondreau, J.M. Boncella

INOR 887. Structure determination of PBP silver complexes. **Y. Cao**, W. Shih, N. Bhuvanesh, O. Ozerov

INOR 888. Cyclopentadienyl pyridazines and oxazines and their applications in energy and advanced electronics. **N.C. Tice**, S. Wild, E. Collins, C. Snyder, D.L. Smith

INOR 889. Chameleonic nature of platinum(II) imidazopyridine complexes. **P. Pinter**, R. Pittkowsky, J. Soellner, T. Strassner

INOR 890. Synthesis & reactivity of novel silyl/silylene pincer cobalt complexes. **J. Zhang**, B.J. Foley, N. Bhuvanesh, M.T. Whited, O.V. Ozerov

INOR 891. Synthesis, characterization and reactivity of pincer-type bis(phosphine)/silylene [P_2Si]Ru complexes. **S. Ma**, J. Zhang, M.T. Whited, D.E. Janzen

INOR 892. Evidence for reversible cyclometalation in alkane dehydrogenation and C-O bond cleavage at iridium bis(phosphine) complexes. **S.M. Chapp**, N.D. Schley

INOR 893. Reactive intermediates in silver-catalyzed nitrene transfer. **C. Mak**, M.G. Campbell

INOR 894. Solution and solid state structures of zerovalent palladium and platinum phosphinoferrocene complexes. **E.A. Kober**, S.H. Schreiner

Section N
Ernest N. Morial Convention Center
Hall D

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S.A. Koch, *Organizer*
5:30–7:30

INOR 895. Mechanistic study of the reaction between KP1019 and serotonin. **L.K. Stultz**, M. Dunbar, V. Krishnan, P. Hanson

INOR 896. Development of novel rhodium-based liver X receptor agonists. **H. Nguyen**, M. Umetani, L. Do

INOR 897. Cytotoxic aldehyde detoxification by organoiridium complexes in cells and zebrafish. **A.H. Ngo**

INOR 898. Design and synthesis of a carboxylate-containing ligand that increases the T1-weighted relaxivity response of a manganese complex to hydrogen peroxide. **T. Hutchinson**, C. Goldsmith

INOR 899. Determining the mechanism by which chromium and bitter melon activates insulin signaling. **P. White**, E. Krol, L.C. Scott, C. Nichols, Z. Krejpcio, J.B. Vincent

INOR 900. Interactions between chromium(III) and DNA. **S. Brown**, J.B. Vincent

INOR 901. Mechanistic insights into intracellular transfer hydrogenation by unprotected organoiridium catalysts. **S. Bose**, L. Do

INOR 902. Synthesis and evaluation of ruthenium complexes with cytotoxicity against cancer cells. **A. Shrestha**, J. Gray, F. Qu, J. Park, Y. Kim, E.T. Papish

INOR 903. Synthesis and cytotoxic properties of organorhenium indomethacinato complexes. **T.V. Hinton**, Y. Zhang, S. Pramanik, S. Mandal

INOR 904. Synthesis, characterization and in vitro antitumor activity of nickel (II) and platinum (II) complexes with some thiophene thiosemicarbazones.. **M.A. Al-Yafeai**, H. Nimir

INOR 905. Synthesis, characterization & in vitro biological activity of Pt(II) and Pd(II) thiosemicarbazone. **Y. Eltayeb**

INOR 906. Effects of small molecule modulators binding to Cu and remodeling the pathway of Cu-catalyzed oxidative stress and aggregation in amyloid $\delta_{(1\text{-}42)}$. **S. Mitra**, S. Chakraborty

INOR 907. Development of iron binding assays to explore structure activity relationships of 3-AP analogs. **S. Plamthottam**, J. Valenzuela, D. Sun, J. Van Valkenburgh, D. Steele, S. Poddar, C.G. Radu, J.I. Zink

INOR 908. NORM's and effects of exogenous agents: Copper promoted NO release from sugar appended thiol DNIC's. **C. Pectol**, C. DeLaney, R.B. Chupik, M.Y. Darensbourg

INOR 909. Organorhenium ibuprofenato, picolinato and nicotinato complexes as anticancer agents. **S. Parnell**, M. Stevenson, Y. Zhang, S. Pramanik, S. Mandal

INOR 910. Photocytotoxicity assessment of a ruthenium(II) polypyridyl complex bearing 2,9-diphenyl-1,10-phenanthroline ligand. N. Mansour, S. Mehanna, M. El Sibai, R.S. Khnayzer, **C. Daher**

Section O
Ernest N. Morial Convention Center
Hall D

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S.A. Koch, *Organizer*
5:30–7:30

INOR 911. Characterization of electron transfer pathways and domain binding pockets in 3-ketosteroid-9β-hydroxylase. **S.R. Soltau**, A. Luiz, P. Patel

INOR 912. Artificial bio-mineralization targeting lanthanide elements. **T. Hatanaka**, A. Matsugami, F. Hayashi, N. Ishida

INOR 913. Formation of myoglobin-nitroso adducts from amine- and nitro-containing drugs. **S. Powell**, B. Wang, X. Yang, V. Herrera, G.B. Richter-Addo

INOR 914. Studies to understand Ti(iV) speciation and transport in the human body.. **J.A. Benjamin-Rivera**, A.D. Tinoco, Y. Delgado, M. Pandrala, A. Vazquez, A. Vazquez

INOR 915. Rate of dissociation of chromium(III) from transferrin under endosomal conditions monitored by EPR. **K.C. Edwards**, M. Lockart, H.H. Kim, M.K. Bowman, J.B. Vincent

INOR 916. Mechanism of oxygen reduction in copper amine oxidases. **S.A. Mills**, K.E. Gazica, M.M. Saugstad

INOR 917. Towards new titanium and vanadium enzymes. O. Peduzzi, A. Paredes, J. Pellegrino, A.J. Reig, **K.M. Buettner**

INOR 918. Electronic effects of a bridging Fe^{II}-Cyanide on $\{Fe(NO)_2\}^{9/10}$ scaffolds for possible linkage isomerization. **M. Quiroz**, P. Ghosh, M.Y. Darensbourg

INOR 919. Synthesis, structure and reactivity of thiolate-bridged $\{Fe(NO)_2\}^9$ dimers with a pendant thiol. **D. Sil**, A. Baxter, M.Y. Darensbourg

INOR 920. Better resolution of Co hyperfine at low frequency: CoEDTA, a model for obtaining Co hyperfine in high spin complexes of biological interest like the transmembrane metal binding site for CzcP. **W.E. Antholine**, M. Ross, B.M. Hoffman, A.C. Rosenzweig

INOR 921. Withdrawn.

INOR 922. Switchable stereoselectivity in monooxygenation of non-native substrates by P450BM3 using decoy molecules. **K. Suzuki**, O. Shoji, J.K. Stanfield, H. Sugimoto, Y. Shiro, Y. Watanabe

INOR 923. Reconstitution of self-sufficient cytochrome P450 with artificial metal complexes. **K. Omura**, Y. Aiba, S. Ariyasu, O. Shoji, H. Sugimoto, Y. Shiro, Y. Watanabe

INOR 924. Simple Zn-scorpionate complexex to test the binding of antimicrobial drugs to Zn containing enzymes. **J. Dewar**, A. Thakur, L. Peterson, W. Eckenhoff

INOR 925. Exploring structural and redox properties of biomimetic models of metal-Aβ binding site in Alzheimer's disease using DFT. **S. Niu**, S.D. Zaric, E.N. Brothers, M.B. Hall

INOR 926. "Beeting" Alzheimer's: Inhibition of Cu^{2+}-β-amyloid mediated oxidation and peroxidation by betanin from sugar beets. **D.C. Cerrato**, L. Ming

INOR 927. Assembling oxygen-evolving complex (OEC) of photosystem II: Design and synthesis of ligands. **J. Prakash**

INOR 928. Synthesis of functional catalysts for CO conversion based on Mo-containing CO dehydrogenase. **M. Foster**, E. Gladhill, L. Nyarko, D. Rokhsana

INOR 929. Models of the molybdenum cofactor: Synthesis and reactivity. **H.H. Varnum**, **V.R. Berke**, D.R. Gisewhite, S.J. Nieter Burgmayer

INOR 930. Short Metallo-peptides and peptoids: A look into the oxidative reactivity. **S. Islam**, C. Tang, D.C. Cerrato, J. Cai, L. Ming

INOR 931. Withdrawn

INOR 932. Structural and reactivity investigation of oxomanganese(IV) and bis(μ-oxo)dimanganese(III,IV) complexes.

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Y. Lee, A.A. Massie, T.A. Jackson

INOR 933. Designed metalloproteins for efficient CO_2 reduction via low valent Fe (I/0) state in aqueous medium. **D. Selvan**, S. Chakraborty

INOR 934. Synthesis and reactivity studies of ene-dithiolate modeling molybdenum cofactor. **N. Nguyen**, D. Gisewhite, S.J. Nieter Burgmayer

INOR 935. Developing TALE proteins as a sensor for detecting pathogens. **K. Gaiko**, M. Kim

Section P
Ernest N. Morial Convention Center
Hall D

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*
5:30–7:30

INOR 936. Fluorometric and colorimetric sensing of citrate with a macrocycle-based dinuclear foldamer in water. M. Rhaman, M.H. Hasan, R. Tandon, **A. Hossain**

INOR 937. Discovery of the novel colorimetric chemosensor for multiple target metal ions Fe^{2+}, Co^{2+}, and Cu^{2+} in a near-perfect aqueous solution: experimental and theoretical studies. **H. Cho**, **M. Yang**, S. Hwang, S. Kim, C. Kim

INOR 938. Development of highly selective turn-on chemosensor for Zn^{2+} in aqueous media and living cells. **D. Yun**, **J. Chae**, J. Jung, J. Kang, C. Rha, C. Kim

INOR 939. Electrochemical investigation of [Ru(saloph)(NO)(Cl)]-type complexes (saloph = N,Nβ-bis-(salicylidene)-o-phenyldiamine, and derivatives). **A. Ramuglia**, A. Fadamin, M.J. Shaw

INOR 940. Ni complexes with redox-active tetradentate ligands: Structures, electrochemistry, and reactivity studies with CO_2. **K.D. Spielvogel**, **J.A. Luna**, **A. Benson**, S.K. Shaw, S.R. Daly

INOR 941. Investigated and calculated solvatochromic characteristics of $MoCl_4$(diimine) anions. **A. Chang**, W.T. Eckenhoff

INOR 942. Metallodithiolate ligands for reversing metal ion induced aggregation of beta amyloid. **E.K. Adams**, M.R. Mackiewicz

INOR 943. Probing valence tautomerism in a cobalt verdazyl coordination compound. C. Kung, S. Fu, D. Chung, **D.J. Brook**

INOR 944. Novel porphyrins bearing phenothiazine pincers to encapsulate fullerenes: Synthesis and complexation study. **K. Jain**, N. Duvva, T. Roy, L. Giribabu, R. Chitta

Section Q
Ernest N. Morial Convention Center
Hall D

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*

5:30–7:30

INOR 945. Synthesis of N-heterocyclic chalcogenone silver complexes. **F. Voges-Haupt**, A. Allen, D. Rabinovich

INOR 946. Synthesis and characterization of model copper(I) and gold(I) thiolate nanoparticle precursor complexes. **C. Tran**, R.J. Papoular, L.E. Marbella, J. Millstone, M. Gembicky, B. Chen, A.T. Royappa

INOR 947. Nitrile reactions of 1,1-bis(diphenylphosphino)ethene dirhenium compounds. **G. Crispin**, **D.J. Esjornson**

INOR 948. Coordination chemistry of *N,N'* azodioxides. **L. Balaraman**

INOR 949. A C_3 symmetric sulfate complex with an *m*-nitrophenyl-functionalized hexaurea receptor. B. Portis, M. Emami Khansari, C. Johnson, D.R. Powell, **A. Hossain**

INOR 950. Exploring new synthetic strategies by using novel manganese carboxylate complexes along with a well-explored ligand, 2-(Hydroxymethyl)-pyridine in the area of polynuclear coordination chemistry. **M.A. Reagan**, A. Saha

INOR 951. Extraordinarily large ferromagnetic coupling ($J \geq 150$ cm^{-1}) via electron delocalization in a heterometallic Mo–Mo–Ni chain complex. **J.A. Chipman**, J.F. Berry

INOR 952. Multicomponent supramolecules in coordination-driven self–assembly: Preparation and photophysical studies. **H. Sepehrpour**, P.J. Stang

INOR 953. Structural and electronic properties of 1,3,6-trisubstituted fulvene chromium complexes. **A. Peloquin**, M. Smith, B. O'Connell, S.K. Adas, G.J. Balaich, S.T. Iacono

INOR 954. Novel colorimetric ligand for the detection of silver (I). **L. Patton**, E. Bosch

INOR 955. Spectroscopic and electronic properties of dissymmetric *trans* Co^{III}-cyclam acetylides and their precursors. **S.D. Banziger**, T. Ren

INOR 956. Synthesis of heteroleptic transition-metal complexes containing azodioxide ligands. **K.A. Emhoff**

INOR 957. Synthesis and coordination chemistry of new Schiff base ligands with hydrogen-bonding groups. **A. Penn**, C. Hamaker

INOR 958. Synthesis and characterization of vanadium(IV), vanadium(V) and iron(III) complexes of perfluoropinacolate ligands. **S.L. Carter**, J.K. Elinburg, J. Nelson, L.H. Doerrer

INOR 959. Structural characterization of a heterobimetallic Zn/La Schiff base complex. **J. Farnsworth**, M. Zeller, E.R. Trivedi

INOR 960. Variation of water cluster motifs in structurally similar Ni(II) complexes: Synthesis, characterization, and thermal analyses. **N. Saraei**, C.S. Mullins, M. Mashuta, R. Buchanan, C. Grapperhaus

INOR 961. Synthesis and characterization of a series of vanadium(IV) complexes with the Kläui ligand. **X. Wu**, C.C. McLauchlan

INOR 962. Molecular characterization of cationic lanthanide complexes containing phosphine oxide. **P.K. Yuen**, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan

INOR 963. Multidentate aminophenols prepared from Mannich condensations. **J.R. Farrell**, M. Bender, J. Kirpas, J. Niconchuk, N. Maniatis, M. Wallace, C.J. Ziegler

INOR 964. Thiol and phenol pendant-arms for cross-bridged tetraazamacrocycle complexes. **P.T. Nguyen**, **D. Jones**, C.C. Jacobsen, T.J. Hubin

INOR 965. Heteroatom-containing bridged azamacrocyles and C-linked bis-azamacrocyles and their coordination complexes. **D. Tresp**, T.K. Ellis, T.J. Hubin

INOR 966. 1,4,7,10,13-pentaazacyclopentadane: Streamlined synthesis and novel transition metal complexes. **F.A. Okorocha**, **A. Shrestha**, A.G. Oliver, J.A. Krause, T.J. Hubin

INOR 967. Ethylene cross-bridged pentaazamacrocycles and their transition metal complexes. **E. Allbritton**, **T.L. Fletcher**, J.A. Krause, A.G. Oliver, T.J. Hubin

INOR 968. Bis-cyclometalated iridium complexes with chelating dicarbene ancillary ligands. **H. Na**, A. Maity, T.S. Teets

INOR 969. Theoretical investigations on radical bridged supramolecular metallacycles toward exploring single molecular magnets. **V. Kuduva Radhakrishnan**, D.I. Alexandropoulos, B.S. Dolinar, K.R. Dunbar

INOR 970. Halogentated formamidinate bridged dirhodium (II,II) complexes as photodynamic therapy based anti-cancer agents. **E. Song**, K.R. Dunbar

INOR 971. Synthesis, spectroscopic characterization and crystal structures of three new zinc(II) complexes of *cis*-1,2-diaminocyclohexane. **M. Monim-Ul-Mehboob**

INOR 972. Highly efficient yellow and red bis-cyclometalated iridium phosphors via ancillary ligand modification. **P. Lai**, T.S. Teets

INOR 973. New bis(amidine) ligands and digold bis(amidine) metalloligands for highly luminescent Group 11 cluster complexes. **O. Ugarte Trejo**, A. Calderón Díaz, N. Siwabut, N. Maya, N. Bhuvanesh, **M. Stollenz**

INOR 974. Role of green chemistry in the synthesis and characterization of several new copper-phenanthroline complexes. **M. Wilk**, R. Johnson, S. Scott, D. Vargas Trujillo, V. Nesterov, M. Omary

INOR 975. Reaction dynamics of the $TeMo_6O_{24}^{6-}$ ion in water. **G.M. Kuhl**, E.M. Villa

INOR 976. Light assisted-oxygen atom transfer from group VI transition metals complexes. **S. Fosshat**, M.B. Chambers

INOR 977. Late transition metal complexes of selenomaltol. **M. Spiegel**, A. Hoogerbrugge, S. Truksa, A. Smith, K.L. Shuford, K. Klausmeyer, P.J. Farmer

INOR 978. Facile metal exchange reactions of ammonium and potassium magnesium dodecaborates. **D.M. Schubert**, M.B. Jacobs

INOR 979. Mononuclear and binuclear Ni complexes with pyridyltriazole ligands. **S. Gao**, T.M. Wheat, J. Theriot, F.R. Fronczek, A.W. Maverick

INOR 980. Investigating multi-electron structure and reactivity with trinuclear μ3-nitride complexes. **A. Su**, J. Teesdale, T. Betley

INOR 981. Novel polymetallonucleosides. **C.M. Mikulski**

INOR 982. Synthesis and characterization of new copper-quinoxaline complexes via solventless and solvent synthetic routes. **K.A. Reyes**, G. Martinez, Y. Faheem, A. Henderson, V. Nesterov, M. Omary

INOR 983. Synthesis and structural characterization of mercury(II) coordination polymers based on 1,2,4,5-tetra(isopropylthio)benzene ligand. **T. Selby-Karney**, S. Kakumanu, J.T. Mague, P. Chandrasekaran

INOR 984. Synthesis, photophysical properties, and DFT studies of Cu(1,7-phen)$(PPH_3)_2PF_6$: An unusual three-coordinate Cu(I) compound and the concept of "inhibited" ligands. **A. Miller**, D.J. Casadonte, A.F. Cozzolino

INOR 985. Metal cluster structure types and electron counts: A survey of the Cambridge Structural Database. **D.H. Johnston**

INOR 986. Comparative studies of Co/Rh/Ni dibenzotetramethylaza[14] annulene (TMTAA) complexes with porphyrin analogs. **S. Dey**, B.B. Wayland, M. Zdilla

INOR 987. Novel aqua and chloro Ru(II) complexes with the tripodal NNN-ligand dipyrido(2,3-a:3',2'-j)phenazine (dpop') and bidentate NN ligands 2,3-di(2-pyridyl)pyrazine(dpp) and 3,6-di(2-pyridyl)tetrazine(dpt) were prepared and characterized.. **R.R. Ruminski**, K. Engstrom, S. Hoover, M. Roe

INOR 988. Molybdenum (VI) amidate complexes: Synthesis and reactivity. **J.M. Smith**, R.K. Thomson

INOR 989. Effects of metal identity on coordination environments and electronic properties in a series of homo- and heterobimetallic complexes of iron and cobalt. **K.M. Gramigna**, R. Mathialagan, S. Kuppuswamy, C.M. Thomas

INOR 990. Designing multicobalt clusters in pursuit of dinitrogen reduction. **M. Eaton**, B.J. Knight, L.J. Murray

INOR 991. Synthesis of chiral amines *via* early transition metal mediated asymmetric reductive hydrogenation of prochiral imines. B. Zhang, R. Josef, J. Bukacek Frazier, L. Kugelmass, A. Atsango, Y. Kim, **J. Tanski**

INOR 992. Metal-Metal bonded complexes supported by artificial sweeteners: Synthesis and characterization of tetra saccharinate and acesulfamate

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complexes of dirhodium(II,II). **S.C. Haefner**

INOR 993. Synthesis and characterization of novel dinitrosyl iron complexes with chelating ligands. **J.M. Grant**, M.W. Jones

INOR 994. Microwave assisted synthesis and characterization of Cr(III) pyrazolate-formate mixed ligand complexes. **J.M. Lopez**, R.G. Raptis

INOR 995. Synthesis and characterization of a novel non-innocent NNP–type pincer ligand and its first-row transition metal complexes. **K. Talukdar**, A. Issa, J.W. Jurss

INOR 996. Computation investigation of carbonyl and ammine gases for the production of solid urea *Via* 5d metal complex. **A. Taylor**, B. Prince

INOR 997. The use of bovine milk for the generation of LacDiNAc (LDN) bearing N-glycans for the chemienzymatic synthesis of Schistosome-type antigenic N-glycans. **K.K. Robinson**

Section R
Ernest N. Morial Convention Center
Hall D

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
5:30–7:30

INOR 998. EPR of lanthanide complexes: exploring the consequences of ligand induced anisotropy. **K. Fisher**, G. Moise, A. Bowen, C. Timmel, S. Faulkner, A. Kenwright

INOR 999. New family of *d/f*-heterobimetallic cationic materials with anion exchange capabilities. **T. Poe**, **M. Polinski**

INOR 1000. Variable coordination motifs of (silyl)anilide ligands on uranium. **A.M. Tondreau**, J.M. Boncella

INOR 1001. Separation of americium from europium using soft donor ligands in ionic liquids. **J. Dehaudt**, N.J. Williams, H. Luo, S. Dai

INOR 1002. Anionic lanthanide complexes containing tetradentate halogen-substituted Schiff base ligands. **P.K. Yuen**, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan

INOR 1003. X-ray diffraction of 1D polymeric lanthanide-transition metal compounds. **P.K. Yuen**, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan

INOR 1004. Novel ionic f-f bimetallic complexes containing salen. **P.K. Yuen**, C.D. Lau, E.M. Yen, A.K. Yuen, W. Chan, H. Chan

INOR 1005. Recent advances in lanthanide chemistry. **R. Beattie**, J.K. Pagano, K. Erickson, S.K. Cope, B. Scott, D.E. Morris, J.L. Kiplinger

INOR 1006. Synthesis, characterization, and photophysical properties of two new organic ligands for the sensitization of lanthanide ions. **D. Tapia**, J.H. Monteiro, A. De Bettencourt Dias

INOR 1007. Development of Gd(III)-based magnetic resonance agents for molecular imaging of hydrogen peroxide and hypoxic tumor conditions. **C. Lynch**, J.O. Massing, E.A. Bajema, K. MacRenaris, T.J. Meade

INOR 1008. Syntheses and crystal structures of lanthanide dithiooxamide complexes. **B.M. Amanda**, E.M. Villa

INOR 1009. Syntheses and crystal structures of lanthanide periodate compounds. **R.N. Colin**, E.M. Villa

INOR 1010. Homoleptic uranium and lanthanide phosphinodiboranate complexes. **T.V. Fetrow**, A.V. Blake, Z. Theiler, S.R. Daly

INOR 1011. CMPO groups and their derivatives to separate rare earth elements. **H.A. Pearson**, **B.G. Wackerle**, **M.L. Hudson**, S.M. Biros

INOR 1012. Solution and solid state structural chemistry of Th(IV) and U(IV)-mono-carboxylates. **N.A. Vanagas**, K.E. Knope

INOR 1013. Identifying actinyl intermolecular interactions of the $U(VI)O_2^{2+}$ cation in coordination compounds. **M. Pyrch**, T. Forbes

INOR 1014. Coordination chemistry and redox-activity of uranium complexes of tetradentate BIAN-type ligands. **J. Niklas**, B.H. Farnum, J.D. Gorden, A.E. Gorden

INOR 1015. Synthesis, structural characterization, and magnetic properties of hexanuclear lanthanide(III) complexes of an extended tritopic picolinic dihydrazide ligand with terminal oxime groups. **S.S. Tandon**, S.D. Bunge, V. Hogan, M. Murugesu

Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 345

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S.A. Koch, *Organizer*
S.A. Toledo, *Presiding*

8:30 INOR 1016. Selective light-driven chemoenzymatic oxytrifluoromethylation. **L.E. Cheruzel**

8:50 INOR 1017. Incorporation of phosphoryl amide moieties to support high valent metal oxido/hydroxido complexes. **V. Oswald**, A. Weitz, E. Hill, N. Sickerman, M.P. Hendrich, A. Borovik

9:10 INOR 1018. Biomimetic reactivity of a family of structural analogues of the resting state of the enzyme nickel-acireductone dioxygenase (Ni-ARD). **S.A. Toledo**, A. Gremillion, J. Jaimes, A.D. Ivan, D. Saldana, A. Sanchez, V. Lynch

9:30 INOR 1019. Design of artificial metalloproteins using Biotin-Streptavidin Technology. **K.R. Miller**, A. Borovik

9:50 INOR 1020. Immobilization of synthetic Cu complexes within a protein host. **D. Brazzolotto**, A. Borovik

10:10 Intermission.

10:20 INOR 1021. Hydroxylation of gaseous alkanes and benzene catalyzed by cytochrome P450BM3 using decoy molecules as a substrate analogue. **O. Shoji**, Y. Watanabe

10:40 INOR 1022. Cellular mapping of carbonic anhydrase and zinc: Towards understanding the bound and labile zinc pool. **R. Mehta**, E.L. Que

11:00 INOR 1023. Modulating intramolecular hydrogen bonding networks in metal complexes to mimic enzyme active sites. **J. Lee**, A. Borovik

11:20 INOR 1024. Three-coordinate iron in an unusual planar iron-sulfur cluster. **D.E. DeRosha**, E. Bill, S. DeBeer, P.L. Holland

11:40 INOR 1025. Withdrawn.

12:00 INOR 1026. Advances in modeling the photosynthetic oxygen evolving complex with geometrically flexible manganese clusters. **M. Zdilla**, S. Vaddypally, S.K. Kondaveeti, I.G. McKendry, D.J. Jovinelli, M.R. Gau, A. Polyak, C. Koellner

Section B
Ernest N. Morial Convention Center
Room 344

Metal-Organic Frameworks: What Are Next?

W. Lin, H. Zhou, *Organizers*
S. Ma, *Organizer, Presiding*
P. McGrier, *Presiding*

8:30 INOR 1027. Porous materials from new framework-forming chemistries. **M.J. Rosseinsky**

9:15 INOR 1028. Expanding the MOF toolkit: Phosphines, arsines and chalcogenides. **S.M. Humphrey**, S. Dunning, R.E. Sikma, R. Riparetti, J. Reynolds, I. Malaestean, J. He

9:45 INOR 1029. Extraction of rare earth elements from geothermal brine solution using magnetic core shell nanoparticles. **P.K. Thallapally**, P. McGrail, J. Liu

10:15 INOR 1030. General and direct method for preparing oligonucleotide-functionalized metal–organic framework nanoparticles. **S. Wang**, C.A. Mirkin

10:35 Intermission.

10:50 INOR 1031. Design and functions of sp^2 carbon covalent organic frameworks. **D. Jiang**

11:20 INOR 1032. Benzobisoxazole-linked covalent organic frameworks. **P. McGrier**

11:50 INOR 1033. Homochiral porous framework as a platform for durability enhancement of molecular catalysts. **F. Xiao**, Q. Sun

12:10 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

D.C. Lacy , C.G. Riordan, J.Y. Yang, *Organizers*
A. Borovik, *Presiding*

8:30 INOR 1034. Chiral recognition of amino alcohols using binuclear Ni(II) complex anion as host. **M. Ray**

8:55 INOR 1035. Cobalt-mediated reactions for sustainable C-H activation processes. **C.E. MacBeth**

9:20 INOR 1036. Coordination polymers and molecular assemblies decorated with hydrogen bonds. **R. Gupta**

9:45 INOR 1037. Developing Single-site organometallic complexes for photochemical water splitting. **D.C. Lacy**

10:10 Intermission.

10:25 INOR 1038. Materials for display applications. **N.S. Radu**, G. Rossi, C.K. Ngai, A. Fennimore

10:50 INOR 1039. Experiments in support of safeguards for aqueous spent nuclear fuel reprocessing. **J.F. Krebs**, C. Pereira

11:15 INOR 1040. Mechanistically driven catalyst design for oxidative coupling reactions. **D. Pappo**

11:40 INOR 1041. Shuttling protons and electrons via the secondary coordination sphere for anion reduction. **J.D. Gilbertson**

Section D
Ernest N. Morial Convention Center
Room 352

Molecular Confinement Effects in Inorganic & Organic Containers

M. Fujita, B.C. Gibb, J.L. Sessler, *Organizers*
M. Hardie, W. Jiang, *Presiding*

8:00 INOR 1042. The inner space environment in coordination chemistry supramolecular clusters. **K.N. Raymond**, C.M. Hong, M. Morimoto

8:30 INOR 1043. Reversible photoswitching in the confinement of coordination cages. **R. Klajn**, D. Samanta

9:00 INOR 1044. Metallo-cages from cyclotriveratrylene-type ligands – chiral self-sorting and speciation control, luminescence and photoswitching behavior. **M. Hardie**, J. Henkelis, V. Pritchard, S. Oldknow, F. Colin, D. Rota Martir, E. Zysman-Colman

9:30 INOR 1045. Guest packing and reactivity within containers assembled via the hydrophobic effect. **B.C. Gibb**

10:00 Intermission.

10:15 INOR 1046. Moelcular discrimination and quantitative detection by luminescent lanthanide-based microporous sensors. **S.M. Humphrey**, S.G. Dunning, A.J. Nunez, R.E. Sikma, M. Moore, A. Steiner, J.L. Sessler

10:45 INOR 1047. Characterization of double and triple decker napthylsalophen complexes with *f*-elements: tunable emission from stacking and extended interactions. **A.E. Gorden**

11:15 INOR 1048. Molecular face-

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rotating polyhedra. **X. Cao**

11:45 INOR 1049. Let's get them talking: Systems of container molecules that work together. **J. Nitschke**

12:15 Concluding Remarks.

Section E
Ernest N. Morial Convention Center
Room 353

Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals

B.C. Melot, J. Vela , *Organizers*
R.L. Brutchey, *Organizer, Presiding*

8:30 INOR 1050. Synthesis and spectroscopy of nanocrystals of compositionally complex haloperovskite semiconductors. S.E. Creutz, M.C. De Siena, E.N. Crites, T.J. Milstein, X. Yuan, J. Zhao, **D.R. Gamelin**

9:10 INOR 1051. Highly dynamic ligand binding and light absorption coefficient of cesium lead bromide perovskite nanocrystals. **J. De Roo**, M. Ibáñez, P. Geiregat, G. Nedelcu, W. Walravens, J. Maes, J.C. Martins, I. Van Driessche, M. Kovalenko, Z. Hens

9:30 INOR 1052. Quantum dot perovskite solar cells: Realizing the best of both worlds for revolutionary optoelectronic applications. **J. Luther**

10:10 Intermission.

10:40 INOR 1053. Colloidal nanocrystals of $APbX_3$ [$A=Cs^+$, $CH_3NH_3^+$, $CH(NH_2)_2^+$, $X=Cl^-$, Br^-, I^-] perovskites with bright photoluminescence spanning the entire visible spectral range. **M. Kovalenko**

11:20 INOR 1054. Computational chemistry to design colloidally stable and trap-free perovskite nanocrystals. S. Boehme, **I. Infante**

11:40 INOR 1055. Single particle luminescence and Raman spectroscopy analyses of lead halide perovskite nanocrystals. **E.A. Smith**, B. Boote, L. Men, D. Freppon, H. Andaraarachchi, J.W. Petrich, J. Vela

Section F
Ernest N. Morial Convention Center
Room 354

Chemistry of Materials: Materials for Energy & Catalytic Applications

C.G. Lugmair, *Organizer*
I. McKendry, C.G. Read, *Presiding*

8:30 INOR 1056. Understanding the role of graphene as an overlayer on nanostructured hematite photoanodes for improved solar water oxidation. **M.P. Cardona**, C. Yang

8:50 INOR 1057. Doping-treated $BiVO_4$ for photocatalytic H_2 fuel production from water. **W. Jo**, K. Gleason, J. Lee

9:10 INOR 1058. High throughput, multi-pH evaluation of earth-abundant pseudo-quaternary metal oxide catalysts for the oxygen evolution reaction. **J. Haber**, D. Guevarra, R. Jones, K. Kan, J. Gregoire

9:30 INOR 1059. Understanding of metal (Ni, Co, Fe) (oxy)hydroxides on graphene as efficient electrocatalysts for water oxidation. **J. He**, R. Miao, W. Zhong, S.L. Suib

9:50 INOR 1060. Cu_2S conformal layer on cubic Cu_2O photocatalytic nanoparticles to increase stability in water splitting reaction. **N.P. Drago**, S. do Amaral Carminati, R.M. Welch, M. Alves de Melo Junior

10:10 Intermission.

10:25 INOR 1061. Withdrawn.

10:45 INOR 1062. The role of inter- and intralayer dopants in 2D layered manganese complexes for cheap and efficient water oxidation catalysis. **I. McKendry**, L. Mohamad, A. Thenuwara, H. Peng, R. Remsing, D.R. Strongin, M. Zdilla

11:05 INOR 1063. Modifying layered manganese oxides for enhanced water oxidation: Turning a cheap, poor catalyst into a cheap, excellent catalyst. **M. Zdilla**, D.R. Strongin, E. Borguet, M.L. Klein, J.P. Perdew, I.G. McKendry, R. Ding, R. Remsing, H. Peng, R.K. Bhullar, L. Mohamad, A. Thenuwara, S.L. Shumlas, Y. Aulin, Q. Kang

11:25 INOR 1064. Operando Raman interrogation of the synthesis and activation of a CoSe HER catalyst. **K.Z. Rinaldi**, A. Carim, N.S. Lewis

11:45 INOR 1065. β-Zirconium phosphate frameworks as supports for active oxygen evolution reaction electrocatalysts. **M. Ramos-Garces**, J. Sanchez, T.F. Jaramillo, J.L. Colon

Section G
Ernest N. Morial Convention Center
Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials
Cosponsored by PHYS
J.L. Dempsey, C. Heyer, E. Leon, G.J. Meyer, *Organizers*
B.H. Farnum, *Presiding*

8:00 INOR 1066. Making solar fuels. **T.J. Meyer**, L. Alibabei, D. Wang, B. Shan, B.J. Sherman, M.V. Sheridan, M.K. Brennaman, A. Nayak, M. Eberhart, Y. Wang, R. Sampaio, L. Troian-Gautier, M.K. Gish, G.J. Meyer, J.M. Papanikolas, K. Wee

8:25 INOR 1067. Moving electrons and protons with visible light-absorbing heteroleptic Cu(I) photosensitizers. B.J. McCullough, B.J. Neyhouse, S.E. Roe, **T.A. White**

8:45 INOR 1068. Modulating electron transfer dynamics at dye-semiconductor interfaces via self-assembled bilayers. **K. Hanson**, J.C. Wang, O. Ogunsolu

9:05 INOR 1069. Chromophore-catalyst assemblies for solar fuels. **K.S. Schanze**, G. Leem, J. Jiang, B. Sherman, Y. Eom, T. Pho, L. Nhon, Z. Morseth, J.R. Reynolds, J.M. Papanikolas, T.J. Meyer

9:25 INOR 1070. Pyridyl-NHC ligated Re and W complexes for the photocatalytic reduction of CO2 to CO and H+ to H2 without photosensitizers. **J.H. Delcamp**, A. Huckaba, H. Shirley, H. Cheema, N. Liyanage, C. Carpenter, R.H. Schmehl, J.W. Jurss, C.E. Webster, N. Hammer

9:45 Intermission.

10:00 INOR 1071. New robust photo- and electrocatalysts for H_2 evolution and CO_2 reduction. **C. Turro**, H.J. Sayre, S. Witt

10:20 INOR 1072. In search for metal-free catalytic motifs for solar fuels. **K. Glusac**

10:40 INOR 1073. Excited state ion-pairs that undergo diffusional excited-state electron transfer. **L. Troian-Gautier**, W. Swords, S.A. Wehlin, M.D. Turlington, E.E. Beauvilliers, G.J. Meyer

11:00 INOR 1074. Light absorption and bond formation from the excited states of metal hydrides. **A.J. Miller**, M.B. Chambers, J.A. Rose, A. Bonn, C.L. Pitman, T. Wong

11:20 INOR 1075. Photocatalytic CO_2 reduction with nickel complexes supported by tunable bipyridyl-*N*-heterocyclic carbenes. X. Su, H. Shirley, J.H. Delcamp, **J.W. Jurss**

11:40 INOR 1076. Homogeneous hydrogen evolving photocatalysis using charge transfer and ligand localized triplet excited states. K. El Roz, M.M. McGoorty, J.E. Yarnell, M. Yang, C.M. Taliaferro, P.M. De La Torre, **F.N. Castellano**

Section H
Ernest N. Morial Convention Center
Room 337

Organometallic Chemistry: New Ligand Platforms

N.S. Radu, *Organizer*
C.H. Larsen, M. Nippe, *Presiding*

8:30 INOR 1077. On-surface synthesis of low coordinate highly reducing metal complexes. **K.G. Caulton**, I.J. Huerfano, A.V. Polezhaev, C. Tempas, T. Morris, D. Wisman, T.S. Rahman, D. Le, S.L. Tait, N. Din

8:50 INOR 1078. Catalyst design for Ti-catalysed [2+2+1] pyrrole formation. **X. See**, I. Tonks

9:10 INOR 1079. Metallocenophane chemistry of the lanthanides: Structure and Magnetism. T. Latendresse, G. Risica, **M. Nippe**

9:30 INOR 1080. Metal-ligand cooperativity with redox-active tetradentate ligands. G. Durgaprasad, J.A. Luna, K.D. Spielvogel, C. Haas, S.K. Shaw, **S.R. Daly**

9:50 INOR 1081. Synthetic strategies to nitrilotriacetamide and tren ligand systems. **D.R. Manke**

10:10 INOR 1082. Impacts of hemilabile moieties in C-H and C-X activation at late transition metals. **E.B. Hulley**, T. Morrow, W. Christman, L. Pap, N. Arulsamy

10:30 INOR 1083. Synthesis of electronically diverse triazole-pyridine ligands: Structure and catalytic activity of corresponding palladium(II) and gold(III) complexes. **C.H. Larsen**, Z.L. Palchak, M.D. Sterling, W.J. Richards, H.M. Ruvalcaba

10:50 INOR 1084. SNAP(O) ligands and their Ru complexes for the practical chemoselective hydrogenation of bio- and oil-derived functionalized esters. **P.A. Dub**, J.G. Schmidt, R.F. Williams, J.C. Gordon

11:10 INOR 1085. Efficient synthesis of imidoylamidines: Liberation of imidoylamidine ligands from heteroleptic nickel (II) complexes. **C.R. Guifarro**, E.V. Rybak-Akimova

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Chemistry of Materials: Metal Organic Frameworks

C.G. Lugmair, *Organizer*
E.D. Bloch, W. Huang, *Presiding*

8:30 INOR 1086. Selective catalytic olefin epoxidation with Mn^{II}-exchanged MOF-5. **A.W. Stubbs**, M. Dinca

8:50 INOR 1087. Withdrawn.

9:10 INOR 1088. Tandem nitrone synthesis using cooperative multifunctional metal-organic framework catalysts. X. Li, B. Zhang, T. Goh, V. Alexander, C. Tsung, L.M. Stanley, **W. Huang**

9:30 INOR 1089. Polyvinylidene fluoride (PVDF)/UiO-66 polymer composite fibers with enhanced catalytic activity towards chemical agents. **D. Dwyer**, D. Cooke, W.E. Bernier, M. Hall, T. Tovar, J. DeCoste, N. Hoffman, N. Dugan, N. Pomerantz, W. Jones

9:50 INOR 1090. MOF catalysis for ethanol to butanol upgrading. **C.N. Neumann**, M. Dinca

10:10 Intermission.

10:25 INOR 1091. Catalytic carbonylation of heterocycles by $Co(CO)_4^-$-incorporated Cr-MIL-101. **H.D. Park**, M. Dinca, Y. Roman-Leshkov

10:45 INOR 1092. Ultramicroporous metal-organic materials with benchmarkselectivities of acetylene/ethylene. Y. Chen, **Z. Zhang**

11:05 INOR 1093. Ethylene dimerization in metal-organic frameworks. **E. Metzger**

11:25 INOR 1094. *Cis*-decalin oxidation as a stereochemical probe of *in-MOF* versus *on-MOF* catalysis. **A.D. Cardenal**, H. Park, D. Powers, C. Chalker

11:45 INOR 1095. Small molecule storage and activation with novel metal-organic materials. **E.D. Bloch**

Section J
Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Applications to Organic Transformations

N.S. Radu, *Organizer*
C. Hahn, J.T. York, *Presiding*

8:30 INOR 1096. Hydroarylation of alkynes catalyzed by late transition metal complexes. **C. Hahn**, B.J. Garcia, C.J. Adams, J. Medina

8:50 INOR 1097. Study of LiX (X=Cl, I, R) in THF: Aggregation states and reactivity, a theoretical study at the QM and QM/MM levels. **A. Milet**, R. David,

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P. Girard, M. Khazri

9:10 INOR 1098. Studies toward enantioenriched molybdenum dearomatization. **J.T. Myers**, P. Shivokevich, S. Dakermanji, J. Smith, C. Trindle, W. Harman

9:30 INOR 1099. Base metal catalyzed, and regioselective hydroboration of pyridines. **S.R. Tamang**, M. Findlater

9:50 INOR 1100. Terminal Rh^{III} methylidene from formal trinuclear oxidative addition of CH_2Cl_2. **T. Morrow**, E.B. Hulley, N. Arulsamy

10:10 INOR 1101. Tethered axial coordination in dirhodium paddlewheel complexes. **A. Darko**, D. Cressy, W. Sheffield, B. Anderson

10:30 INOR 1102. Investigating the binding and electrophilic activation of ethylene by group 12 metal ions. **J.T. York**

10:50 INOR 1103. Kinetics and mechanism of iron-catalyzed transfer hydrometallation. **B.V. Popp**

11:10 INOR 1104. Catalytic photoredox arene and heteroarene C-C bond-forming reactions driven without sacrificial reagents by tungsten-alkylidyne chromophores. **H.B. Vibbert**, M.D. Hopkins

Section K
Ernest N. Morial Convention Center
Room 335

Organometallic Chemistry: Applications to Materials & Polymer Science

N.S. Radu, *Organizer*
T.W. Hudnall, *Presiding*

8:30 INOR 1105. Synthesis of diverse C-H bond activated nonmetallocene lanthanides as a versatile tool for functionalized homo- and blockcopolymers *via* group-transfer polymerization. **F. Adams**, B. Rieger

8:50 INOR 1106. Substitution effects in highly syndioselective styrene polymerization catalysts based on single-component allyl *ansa*-lanthanidocenes: A theoretical study. **E. Louyriac**, L. Maron

9:10 INOR 1107. Electrophilic carbenes: Tales of main group chemistry, radicals, and photochemistry. **T.W. Hudnall**, T.A. Perera, R.N. Arias, M.B. Gildner

9:30 INOR 1108. Synthesis, characterization and applications of highly modular polyphosphonates. **T.R. Totsch**, G. Gray

9:50 INOR 1109. New complexes for nickel-catalyzed olefin polymerization. **A. Kocen**, M. Brookhart, O. Daugulis

10:10 INOR 1110. Synthesis of hyperbranched polyethylene with triazolecarboxamidate supported nickel complexes. **D. Xiao**, L. Do

10:30 INOR 1111. *In situ* Lewis acid recruitment effects on (b)py-appended late transition metal catalyzed ethylene polymerization. **A. Smith**, I. Tonks

10:50 INOR 1112. Rhodium-catalyzed dehydropolymerization of arsine boranes. **B. Ackley**, R. Waterman

11:10 INOR 1113. Photochemical reactions of Ru precursors for photoassisted chemical vapor deposition. **C.R. Brewer**, O.M. Hawkins, B. Salazar, A.V. Walker, L. McElwee-White

Radiopharmaceutical Chemistry

Fluorine

Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Confinement: Clay Mineral Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and INOR

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

R&D in the Chemical Catalysis for Bioenergy Consortium
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Catalysis & Surface Science Science Applied to the Destruction of Threat Agents

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 345

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
J.L. Brumaghim, J.R. Jeitler, *Presiding*

1:30 INOR 1114. Complexes of 2,6-pyridinedicarboxylate: Understanding the complex chemistry of a simple ligand. **J.R. Jeitler**, M. Jeitler, S. Patberg, E. Schafhausen

1:50 INOR 1115. Coordination sphere effects on unusually large zero field splitting and slow magnetic relaxation in trigonally symmetric 3d molecules. **K. Schulte**, V. Kuduva Radhakrishnan, K.R. Dunbar

2:10 INOR 1116. Effects of second coordination sphere on the properties and reactivity of Mn(III)–oxido complexes. **S. Barman**, J.R. Jones, C. Sun, A. Borovik

2:30 INOR 1117. Anisotropic exchange in polynuclear complexes containing Mo^{III}. **D.K. Kempe**, T.J. Woods, K. Schulte, H. Zhao, M.R. Saber, K.R. Dunbar

2:50 INOR 1118. Homo- and heterobimetallic complexes supported by an unsymmetric redox-active ligand. **C. Hess**

3:10 Intermission.

3:20 INOR 1119. Copper-thione complexes are truly complex: Redox and sulfur extrusion reactions. J.M. Murphy, C.D. McMillen, **J.L. Brumaghim**

3:40 INOR 1120. Rhenium metal-metal bonded fluoro complexes. **S. Mariappan Balasekaran**, A.P. Sattelberger, A. Hagenbach, F. Poineau

4:00 INOR 1121. Preparation and structure of lanthanide complexes coordinated to FcCOO and DTBbpy ligands. **N. Johns**, S. Mariappan Balasekaran, A. Chang, P.K. Bhowmik, F. Poineau

4:20 INOR 1122. Employment of non-innocent ligands in transition metal coordination chemistry. **D.I. Alexandropoulos**, B.S. Dolinar, V. Kuduva Radhakrishnan, K.R. Dunbar

Section B
Ernest N. Morial Convention Center
Room 344

Electrochemistry

B.L. Lucht, *Organizer*
M. Zdilla, *Presiding*

1:30 INOR 1123. Highly conductive molecular electrolytes for safer lithium batteries designed through use of the Pearson hard-soft acid-base concept. **M. Zdilla**, S.L. Wunder, P.R. Chinnam, B. Fall, M. Van Vliet, A. Jalil, R.N. Clymer, A. Venkatnathan, P. Prakash, J. Aguirre

1:50 INOR 1124. Crystalline-amorphous Co@CoO core-shell heterostructures for efficient electro-oxidation of hydrazine. **X. Yan**, Y. Liu, J. Lan, Y. Yu, J. Murowchick, X. Yang, Z. Peng

2:10 INOR 1125. Benchmarking the effects of surface ligands on CoP for the hydrogen evolution reaction. **D. Ung**, B.M. Cossairt

2:30 INOR 1126. Pollutant detection with electrochemical biosensors. **A.L. Furst**, M.B. Francis

2:50 Intermission.

2:55 INOR 1127. Reduction potential and stability trends in heterobimetallic complexes containing trivalent redox-inactive cations. **A. Kumar**, V. Day, J.D. Blakemore

3:15 INOR 1128. Single-electron redox chemistry of [Cp*Rh] enabled by a nitrated bipyridine ligand. **W. Moore**, W.C. Henke, D. Lionetti, V. Day, J.D. Blakemore

3:35 INOR 1129. The electrochemical quartz crystal microbalance as a probe of molecular catalyst homogeneity. **D.J. Sconyers**, J.D. Blakemore

3:55 INOR 1130. Catalysis of the oxygen evolution reaction in strongly acidic electrolytes with earth-abundant crystalline nickel-manganese antimonate. **I.A. Moreno-Hernandez**, C.A. MacFarland, C.G. Read, K. Papadantonakis, B.S. Brunschwig, N.S. Lewis

4:15 INOR 1131. Scalable redox-active coordination network films toward molecular devices. **M. Haga**, K. Yoshikawa, D. Motoyama, H. Ozawa

Section C
Ernest N. Morial Convention Center
Room 343

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Andrew S. Borovik

C.G. Riordan, J.Y. Yang, *Organizers*
D.C. Lacy , *Organizer, Presiding*

1:30 INOR 1132. Recent advances in the +2 oxidation state chemistry of the rare-earth and actinide metals. **W.J. Evans**

1:55 INOR 1133. Cytochrome P450 compound I: A direct link between electron donation and reactivity. **M. Green**

2:20 INOR 1134. Further studies in ligand non-innocence: Managing electrons and protons. **A.F. Heyduk**, K. Rosenkoetter, B. Charette, C. Ramirez

2:45 INOR 1135. Electrifying the secondary coordination sphere: Proximal cations and their effect on redox reactivity. **J.Y. Yang**, A. Reath, T. Chantarojsiri

3:10 Intermission.

3:25 INOR 1136. Structural biology of redox partner binding: Simple and complicated. **T.L. Poulos**

3:50 INOR 1137. The 6,6′-biazulenic motif: From unusual polyelectrochromism to molecular nanostructures with remarkably high redox capacity. **M.V. Barybin**

4:15 INOR 1138. What do molecules want? **C.B. Aakeroy**

4:40 INOR 1139. Nickel-dioxygen complexes: Synthesis, structure and reactivity. **C.G. Riordan**

5:05 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 352

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
I. Hartenbach, E.M. Villa, *Presiding*

1:30 INOR 1140. Isolation of lanthanide cryptate complexes by ligand rearrangement and encapsulation. **D.N. Huh**, J.W. Ziller, W.J. Evans

1:50 INOR 1141. Facile linking of lanthanide cations with soft metals *via* thiosulfate. **E.M. Villa**, E.Z. Dalton

2:10 INOR 1142. Weak field ligands in *f*-element chemistry. **H.S. La Pierre**, N.T. Rice, T.P. Gompa, B.J. Yik, L.M. Aquirre-Quintana

2:30 Intermission.

2:40 INOR 1143. Molecular approaches to rare earth separations: Tuning ligand electronics for a greener system. **B.E. Cole**, I.B. Falcones, T. Cheisson, B.C. Manor, P.J. Carroll, E.J. Schelter

3:00 INOR 1144. Prism inside: Lanthanide chloride oxidotungstates and -molybdates of the formula $Ln_3Cl_3[MO_6]$ (Ln = La – Nd, Sm – Er; M = Mo, W). K.V. Dorn, **I. Hartenbach**

3:20 INOR 1145. Structural chemistry of Ce(IV), Th(IV), and U(IV) complexes

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isolated from acidic aqueous media. **J.N. Wacker**, O.C. Stewart, Jr., K.E. Knope

3:40 Intermission.

3:50 INOR 1146. An exploration of the lanthanide fluorite structure, MO2 (Ce, Pr, and Tb) by microRaman. **J.T. Stritzinger**, G. Goff, K. Boland

4:10 INOR 1147. Reactivity of the isolated divalent lanthanide complexes $\{Ln[N(SiMe_3)_2]_3\}^{1-}$ with small molecules: CO, CO_2, N_2. **A. Ryan**, J.W. Ziller, W.J. Evans

4:30 INOR 1148. Ferrocene-based redox switches for reversible single-molecule magnet behaviour in dysprosium(III) and erbium(III) bis-diamidoferrocene complexes. **C.M. Dickie**, A.L. Laughlin, J.D. Wofford, N. Bhuvanesh, M. Nippe

4:50 INOR 1149. Formation of thorium and uranium – phosphorano–stabilized carbene. **P. Rungthanaphatsophon**, L. Maron, J.R. Walensky

Section E
Ernest N. Morial Convention Center
Room 353

Inorganic Chemistry of Lead Halide Perovskites: Insights from Fundamentals

R.L. Brutchey, B.C. Melot, *Organizers*
J. Vela , *Organizer, Presiding*

1:30 INOR 1150. Interfaces, cations, and carrier dynamics in halide perovskites. **D.S. Ginger**

2:10 INOR 1151. Rationalizing the size-dependent Stokes shift in $CsPbBr_3$ nanocrystals. **M.C. Brennan**, J.E. Herr, T.S. Nguyen-Beck, J. Parkhill, M.K. Kuno

2:30 INOR 1152. Enhancing the sensitivity of ^{207}Pb solid-state NMR spectroscopy for characterization of organolead halide perovskites. M.P. Hanrahan, B. Rosales, L. Men, J. Vela , **A.J. Rossini**

3:10 Intermission.

3:40 INOR 1153. Is mesoscopic TiO_2 in perovskite solar cells an innocent bystander or a direct participant. R.A. Scheidt, E. Kerns, **P.V. Kamat**

4:20 INOR 1154. Transition path of organic cation induced anomalous photoluminescence in hybrid lead perovskites from real-time single crystal neutron diffraction. **X. Wang**, B. Yang, K. Xiao

4:40 INOR 1155. Synthesis and optical properties of 2D halide perovskites. **W.A. Tisdale**

Section F
Ernest N. Morial Convention Center
Room 354

Chemistry of Materials: Materials for Energy & Catalytic Applications

C.G. Lugmair, *Organizer*
R. Coridan, O. Gunaydin-Sen, *Presiding*

1:30 INOR 1156. Search, discovery, and properties of ternary nitrides. **S. Lany**, A. Holder, W. Sun, E. Arca, S. Bauers, G. Ceder, A. Zakutayev

1:50 INOR 1157. Selective metal oxide atomic layer deposition: Toward precision few-atom clusters synthesis. D. Cao, J. Emery, M. Pellin, **A.B. Martinson**

2:10 INOR 1158. Physical and chemical applications of photodoping in electrodeposited cuprous oxide thin films. J. Lowe, **R. Coridan**

2:30 INOR 1159. Synthesis of fluorinated tungsten (VI) oxo-alkoxide complexes as precursors for the chemical vapor deposition of WO_x. **N. Ou**, D.C. Bock, L. McElwee-White

2:50 Intermission.

3:05 INOR 1160. The effect of different molecular weight and catalyst on ammonia borane: Polvinylpyrrolidone hydrogen storage composites. **O. Gunaydin-Sen**, R. Seemaladinne, S. Pati, K. Kharel, A. Bafana, A. al-Wahish, E. Wujcik

3:25 INOR 1161. Manganese(I) and rhenium(I) molecular CO_2 reduction catalysts heterogenized on gold electrodes at bipyridine sites in Rh(I) 5,5β-diisocyanide-2,2β-bipyridine coordination polymers. **G. Lee**, C.P. Kubiak

3:45 INOR 1162. Microwave-assisted hydrothermal carbonization of waste plant materials: An approach for improving their energy properties. **S. Elaigwu**

Section G
Ernest N. Morial Convention Center
Room 210

PCET PhotoCatalysis with Inorganic Molecules & Materials
Cosponsored by PHYS
C. Heyer, E. Leon, G.J. Meyer, *Organizers*
J.L. Dempsey, *Organizer, Presiding*

1:30 INOR 1163. Multiple proton transfers coupled to a single electron transfer in benzimidazole-phenol derivatives. S. Mora, E. Odella, B. Wadsworth, M.T. Huynh, G.F. Moore, S. Hammes-Schiffer, D. Gust, T.A. Moore, **A.L. Moore**

1:55 INOR 1164. Switching the mechanism: Proton-coupled electron transfer reactivity of a tungsten hydride complex. **J.L. Dempsey**, T. Huang

2:15 INOR 1165. Mechanistic roles of hydrogen bonding interactions in photoinduced PCET. **D.E. Polyansky**, S. Lymar, M. Ertem

2:35 INOR 1166. Innovating bimetallic active sites for small-molecule catalysis. **C. Lu**, R. Cammarota, M.V. Vollmer, S.P. Desai, J. Vitillo, J. Xie, J. Ye, L. Gagliardi

2:55 INOR 1167. Excited State PT, ET and PCET in Hydroxybipyridine Ru(II) Complexes in Nonaqueous solution. K. Martinez, M. Esposito, J.J. Paul, **R.H. Schmehl**

3:15 Intermission.

3:30 INOR 1168. Toward light-driven multiple-electron-coupled proton-transfer (ECPT) reactions. S. Luo, C. Sanborn, W. White, L. Renna, **S. Ardo**

3:50 INOR 1169. Excited-state proton transfer in transition metal compounds. **R. Sampaio**, R.M. O'Donnell, G. Li, G.J. Meyer

4:10 INOR 1170. Free energy relationships in the formation of cobalt hydrides through PCET. **D. Kurtz**, N. Elgrishi, B. Kandemir, W. Howland, J.L. Dempsey

4:30 INOR 1171. PCET branch-points in CO_2-to-fuels catalysis. **Y. Surendranath**, A. Wuttig, Y. Yoon, S. Khan, M. Schreier

4:50 INOR 1172. Charge transfer through metal oxides on semiconductors for hydrogen evolution. **M.J. Rose**, J. Seo, H. Kim, R. Pekarek

5:10 INOR 1173. Probing the elementary steps of PCET catalysis. R. Lomoth, T. Liu, S. Wang, S. Ott, **L. Hammarstrom**

Section H
Ernest N. Morial Convention Center
Room 211

Chemistry of Materials: Metal Organic Frameworks

C.G. Lugmair, *Organizer*
C. Mulzer, I. Stassen, *Presiding*

1:30 INOR 1174. O_2 electroreduction catalyzed by conductive metal-organic frameworks. **E. Miner**, M. Dinca

1:50 INOR 1175. Signature of metallic behavior in the metal-organic frameworks M_3(hexaiminobenzene)$_2$ (M = Ni, Cu). **J. Dou**, M. Dinca

2:10 INOR 1176. Vertical and lateral charge transport in ultrathin films of metal organic frameworks. **C. Marti-Gastaldo**

2:30 INOR 1177. Tunable, high single crystal conductivity in a permanently porous metal-organic framework. **L. Xie**, L. Sun, R. Wan, S. Park, J. DeGayner, C.H. Hendon, D. Harris, M. Dinca

2:50 INOR 1178. Synthesis and electromagnetic properties of square-symmetry π-conjugated metal-organic frameworks. **I. Stassen**, M. Dinca

3:10 Intermission.

3:25 INOR 1179. Charge transfer within MOF: The role of polar node. **P. Deria**

3:45 INOR 1180. Systematic study of conductive metal-organic frameworks as electrocatalysts for oxygen reduction reaction. **L. Wang**, E. Miner, M. Dinca

4:05 INOR 1181. Synthesis and characterization of novel palladium- and platinum-based metal-organic frameworks for thermoelectrics. **M.C. So**, N.D. Mackie, S. Yoon, V. Cherrette, Y. He, V. Stavila, A.A. Talin, J. Llinas, M. Allendorf, K.L. Mulfort

4:25 INOR 1182. Design and synthesis of highly stable metal organic frameworks with predesigned interactions with light. **W. Newsome**, G.S. Pour, R. Ly, J. Cordova, F.J. Uribe-Romo

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Organometallic Chemistry: Applications to Organic Transformations

N.S. Radu, *Organizer*
J.M. Camara, *Presiding*

1:30 INOR 1183. New fluoro-organometallic chemistry of nickel and copper. **D.A. Vicic**, M. Kosobokov, S. Yu

1:50 INOR 1184. Carbon–fluorine bond formation from copper(I) vinyls: Synthesis of fluoroalkenes from alkynes. **A. Jordan**, P.K. Thompson, J.P. Sadighi

2:10 INOR 1185. Copper-catalyzed P–C cross-coupling for the synthesis of secondary phosphines and related ligands.. M. Frik, A.L. Haber, E.B. Schiff, **J.M. Camara**

2:30 INOR 1186. Cobalt complexes of tripodal ligands with mixed P, N donors: Applications for catalytic dehydrogenative coupling reactions. **K. Ding**, S. Xu, K. Paudel, B. Pandey, D.L. Tyer

2:50 INOR 1187. Immobilization of molecular nickel cross-coupling catalyst on oxide supports via atomic layer deposition. **R. Key**, A.K. Vannucci

3:10 INOR 1188. How to predict reactivity on organometallic reactions from user-friendly computational tools. **A. Poater**

3:30 INOR 1189. Multiple aromatic C-H bond activations by a dirhenium carbonyl complex. **P. Dhull**, R.D. Adams

3:50 INOR 1190. Toward absolute measurements of Pd(π-arene) C–H acidity. **W. Christman**, T. Morrow, N. Arulsamy, E.B. Hulley

4:10 INOR 1191. Homogeneous (transfer) hydrogenation for the selective conversion of β,β-unsaturated aldehydes. **J.G. De Vries**, R. Farrar-Tobar, P. Puylaert, B. Stadler, S. Hinze

Section J
Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N.S. Radu, *Organizer*
A.M. Tondreau, *Presiding*

1:30 INOR 1192. 1st row transition metals supported by dianionic PNP-chelate ligands; Reactivity and electronic structure. **A.M. Tondreau**, N.H. Anderson, J.M. Boncella

1:50 INOR 1193. Nickel complexes bearing the ^{iPr}PN^{H}P and ^{tBu}PN^{H}NOP ligands: Synthesis, characterization, and subsequent reactivity. **N. Anderson**, A.M. Tondreau, J.M. Boncella

2:10 INOR 1194. Photoinduced electron transfer reaction of bis-cyclometalated iridium complexes with β-diketiminate ancillary ligands. **J. Shon**, T.S. Teets

2:30 INOR 1195. Monometallic and bimetallic platinum complexes with fluorinated β-diketiminate ligands. **K. Choung**, T.S. Teets

2:50 INOR 1196. Phosphorescent platinum(II) complexes with mesoionic NHC ligands – tuning the excited state. **J. Soellner**, T. Strassner

3:10 INOR 1197. Synthesis and reactivity of reduced CCC-NHC rhodium pincer complexes. **J. Denny**, R.W. Lamb, C.E. Webster, T.K. Hollis

‡*Cooperative Cosponsorship*

3:30 INOR 1198. CCC-NHC pincer iron complexes: Synthesis of bis CCC-NHC complexes and ligand functionalization after complexation. **J. Cope**, R.W. Lamb, J. Denny, C.E. Webster, T.K. Hollis, B. Donnadieu

3:50 INOR 1199. Synthesis, characterization, and photophysics of CCC-NHC pincer Platinum complexes. **M. Zhang**, S. Autry, V. Dixit, E.V. Dornshuld, J. Denny, N. Hammer, C.E. Webster, T.K. Hollis

4:10 INOR 1200. Accessing reactive oxo intermediates: Oxidation of a CCC-NHC-Pt complex. **G.M. Lang**, J. Denny, V. Dixit, C.E. Webster, T.K. Hollis

4:30 INOR 1201. Boryl participation in H-X cleavage facilitated by (PBP)Ir and (PBP)Rh complexes. **Y. Cao**, W. Shih, N. Bhuvanesh, O. Ozerov

Section K
Ernest N. Morial Convention Center
Room 335

Main Group Chemistry

T.W. Hudnall, *Organizer*
A.F. Cozzolino, *Presiding*

1:30 INOR 1202. Novel Cu(I)- and Co(II)-Sb complexes: Magnetic properties,luminescence, and catalysis. **L. Taylor**

1:50 INOR 1203. Advances in the synthesis of Te, N-containing heterocycles: Potential building blocks for supramolecular frameworks. N.L. Silar, B.A. Larson, F.R. Fronczek, **T. Junk**

2:10 INOR 1204. Metalated ylides: Unique donor ligands for main group chemistry. **V.H. Gessner**

2:30 INOR 1205. Flexible nature of the carbodiphosphorane, $C(PPh_3)_2$, and its reactivity towards main group alkyl complexes. **P. Quinlivan**, G. Parkin

2:50 INOR 1206. Development of hypervalent 10–P–3 compounds for use as transition metal surrogates: The journey continues.... **M. Cain**

3:10 INOR 1207. Controlling molecular recognition and self-assembly with pnictogen(III) secondary bonding interactions in the solid and solution states. S. Moaven, J. Qiu, **A.F. Cozzolino**

3:30 INOR 1208. Cationic antimony containing compounds as Lewis acid catalysts for transfer hydrogenation reactions. **M. Yang**, M. Hirai, F.P. Gabbaï

3:50 INOR 1209. Platinumβtrifluorostiborane complexes as carbophilic catalysts: Activation by fluoride anion abstraction from the trifluorostiborane Z-type ligand. **D. You**, H. Yang, S. Sen, F.P. Gabbai

4:10 INOR 1210. Understanding Te and Sb separations in support of targeted Auger therapy using X-ray absorption spectroscopy. **S. Bone**, K.T. Bennett, M.G. Ferrier, B.W. Stein, J. Engle, S.A. Kozimor

4:30 INOR 1211. Withdrawn.

4:50 INOR 1212. Synthesis, spectroscopic properties and biological activities of spiro-4-bromobenzylaminophosphazenes. **N. Guven Kuzey**, **N. Asmafiliz**, L. Acik, T. Hokelek

5:10 INOR 1213. Phonon-induced superstructures in layered titanium-oxypnictides superconductors. **R. Maezono**, K. Nakano, K. Hongo

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde
Sponsored by I&EC, Cosponsored by INOR‡

Radiopharmaceutical Chemistry

Carbon-11 & Radionuclide Production

Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

Unconventional Catalysis Targeting Stable Molecules
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Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Carbonates, Phosphates & Rare Earth Elements

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Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
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Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Photocatalytic Approaches

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

WEDNESDAY EVENING

Fluid-Solid Interfacial Phenomena at the Nexus of Energy & Geochemistry Research: A Symposium in Honor of David J. Wesolowski

Sponsored by GEOC, Cosponsored by COLL, ENFL, ENVR and INOR

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments
Sponsored by GEOC, Cosponsored by ENVR and INOR

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Sponsored by GEOC, Cosponsored by ENVR and INOR

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 345

Chemistry of Materials: Metal Organic Frameworks

C.G. Lugmair, *Organizer*
P.J. Milner, J.P. Vizuet, *Presiding*

8:30 INOR 1214. Record-setting sorbents for water and ammonia: Engineering capacity, kinetics, and stability. **A.J. Rieth**, M. Dinca

8:50 INOR 1215. Cracking down on vapochromic materials: Vapor induced stress in gas sensing platinum salts. **A.E. Norton**, S. Taylor, J.A. Krause, W.B. Connick

9:10 INOR 1216. Holmium-based metal-organic framework for gas separations and cancer therapy. **J.P. Vizuet**, K.J. Balkus

9:30 INOR 1217. Understanding the mechanism of carbon dioxide uptake by a photoresponsive MOF. **R. Poloni**, C. Yang, A. Charaf Eddin, L. Lin

9:50 INOR 1218. Diamine-appended metal-organic frameworks for carbon dioxide capture from fossil fuel-fired power plants. **P.J. Milner**, R. Siegelman, J. Martell, A. Forse, M.I. Gonzalez, T. Runcevski, D. Gygi, J.A. Reimer, J.R. Long

10:10 Intermission.

10:25 INOR 1219. Adsorption and sensing properties of metal-organic frameworks with mixed organic ligands. **W. Sun**

10:45 INOR 1220. Exploring the effect of ligand design on porphyrin metal-organic framework separation performance. **H. Rubin**, M.M. Reynolds

11:05 INOR 1221. Withdrawn

11:25 INOR 1222. Gas separations in a metal–organic framework featuring exposed vanadium(II) sites. **D. Reed**, D. Jaramillo, J.R. Long

11:45 INOR 1223. In-situ characterization of adsorbates in nanoporous materials with infrared spectroscopy. **H. Jiang**, J. Long

Section B
Ernest N. Morial Convention Center
Room 344

Solid-State Inorganic Chemistry

C.G. Lugmair, *Organizer*
V. Poltavets, *Organizer, Presiding*

8:30 INOR 1224. Structural and optical properties of two new non-centrosymmetric compounds: $MgSiAs_2$ and $Mg_3Si_6As_8$. **K. Woo**, J. Wang, K. Lee, J. Dolyniuk, K. Kovnir

8:50 INOR 1225. Withdrawn

9:10 INOR 1226. Polyamorphism induced multi-level electronic states in phase change $K_2Sb_8Se_{13}$. **M.S. Islam**, L. Peng, L. Zeng, C. Malliakas, D. Chung, B. Buchholz, T. Chasapis, R. Li, K. Chrissafis, J. Medvedeva, G. Trimarchi, M. Grayson, T.J. Marks, M.J. Bedzyk, R. Chang, V. Dravid, M. Kanatzidis

9:30 INOR 1227. Utilizing heterostructural alloying to design improved piezoelectrically active nitrides. **S. Millican**, K. Talley, C. Musgrave, G. Brennecka, A. Holder

9:50 Intermission.

10:05 INOR 1228. Withdrawn.

10:25 INOR 1229. Cu_2IrO_3: Toward the quantum spin liquid phase in honeycomb iridates. **M. Abramchuk**, C. Ozsoy-Keskinbora, J.W. Krizan, K.R. Metz, D.C. Bell, F. Fallah Tafti

10:45 INOR 1230. Synthesis of β-Fe2O3 hollow spheres: photonic crystal mimics. **A.M. Morey**, S.T. Iacono

11:05 INOR 1231. Real-time observation of nanoscale manipulation of metal oxide phase transformations using *in situ* transmission electron microscopy. L. Yu, B.M. Hudak, R. Han, G. Waetzig, S. Depner, X. Sang, J. Liu, A. Talapatra, R. Arroyave, K. Page, S. Banerjee, **B. Guiton**

11:25 INOR 1232. Investigation of the effect of rare-earth substitution on the Debye temperature of YAG:Ce^{3+} and BAM:Eu^{2+}. **A.C. Duke**, W. Zeier, J. Brgoch

Section C
Ernest N. Morial Convention Center
Room 343

Nanoscience

B.G. Trewyn, *Organizer*
A.A. Marti, *Presiding*

8:30 INOR 1233. Flow synthesis of MOF nanoparticles in microfabricated reactors. **K. He**, K. Yeung

8:50 INOR 1234. High efficiency and long-term intracellular activity of an enzymatic nanofactory based on metal-organic frameworks. **X. Lian**, H. Zhou

9:10 INOR 1235. Grafting organic functionalities to boron-nitride nanotubes using Billups-Birch reaction. **A.A. Marti**, C. de los Reyes, A. Smith, K. Walz, M. Pasquali

9:30 INOR 1236. Polyarylboranes: Unexpected reactivity from some of the most stable ions. **M.W. Lee**, T. Wang

9:50 INOR 1237. Phase directing ability of an ionic liquid solvent for the synthesis of colloidal Ni_2P nanocrystals. **E.J. Roberts**, C.G. Read, N.S. Lewis, R.L. Brutchey

10:10 INOR 1238. Synthetic phase control over colloidal nickel sulfide nanocrystals. **G. Barim**, R.L. Brutchey

10:30 Intermission.

10:30 INOR 1239. Dynamic nature of thiolate monolayer in $Au_{25}(SR)_{18}$ nanoclusters. **G. Salassa**, A. Seles, F. Mancin, T. Bürgi

10:50 INOR 1240. Exploiting surface plasmon resonance in Au/ZnO photocatalysts for the selective oxidation of phenols. F. Lin, B.E. Cojocaru, **L.W. Colaciello**, C.A. Cadigan, C. Tian, M.N. Grecu, H. Xin, S. Vyas, V.I. Parvulescu, R.M. Richards

11:10 INOR 1241. Withdrawn.

11:30 INOR 1242. Cyclohexane oxidation over rock-salt structured metal oxides as catalysts. **Q. Yao**, C.A. Cadigan, A.R. Corpuz, G. Jeong, R.

‡*Cooperative Cosponsorship*

Bhattacharjee, R.M. Richards

11:50 INOR 1243. Microwave synthesis of Ir-based binary alloy nanoparticles and catalytic properties for hydrogenation. **H. Guo**, H. Li, K. Javis, H. Wan, P. Kunal, S. Dunning, D.S. Fernandez, S.M. Humphrey, G.A. Henkelman

Section D
Ernest N. Morial Convention Center
Room 352

Main Group Chemistry

T.W. Hudnall, *Organizer*
C. Chiu, *Presiding*

8:00 INOR 1244. Reduction of aryl(hydro)boranes: Versatile bond-formation reactions. **T. Kaese**, M. Wagner

8:20 INOR 1245. Withdrawn.

8:40 INOR 1246. Borafluorenes with ultra-large Stokes shifts. **J. Cassidy**, P.A. Rupar, I. Adams, M. Smith

9:00 INOR 1247. Utilization of BODIPY dyes to introduce redox chemistry into main group complexes. **Z.M. Heiden**, I.A. Kieffer, R.J. Allen, J. Deobald

9:20 INOR 1248. One step conversion of ptassium organotrifluoroborates to metal organoborohydrides. **E.R. Abbey**

9:40 INOR 1249. Boron containing radicals. M. Chung, H. Tsai, W. Liu, **C. Chiu**

10:00 INOR 1250. Microwave-promoted reactions of the CB_{11}^- carborane anion. **M.A. Juhasz**

10:20 INOR 1251. Lewis superacidic ionic liquids with borenium cations. **M. Swadzba-Kwasny**, S. Coffie, J.M. Hogg, F. Coleman, A. Ferrer-Ugalde, J.D. Holbrey

10:40 INOR 1252. Alkyl groups as electron density donors in π-hole bonding. **J. Echeverria**

11:00 INOR 1253. Lanthanum catalyzed heterodehydrocoupling of silanes with amines. **M. Cibuzar**, R. Waterman

11:20 INOR 1254. Facile access to organometallic heavy alkaline earth metal species using environmentally friendly redox transmetallation protolysis (RTP). Y. Takahashi, A.Y. O'Brien, G.B. Deacon, P.C. Andrews, M. Wolf, A. Torvisco, **M.M. Gillett-Kunnath**, K. Ruhlandt-Senge

11:40 INOR 1255. Reductive CO_2 homologation: C-C homocoupling and asymmetric carbon generation. **S. Bontemps**

Section E
Ernest N. Morial Convention Center
Room 353

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
M.P. Marshak, F. Poineau, *Presiding*

8:30 INOR 1256. Speciation and reactivity of heptavalent technetium in strong acids. **F. Poineau**

8:50 INOR 1257. Molecular magnets utilizing anisotropic coupling with 4d and 5d cyanometallate compounds. **F.J. Birk**, D. Pinkowicz, K.R. Dunbar

9:10 INOR 1258. An investigation into the reactivity profile of high-spin iron hydride clusters. **B.J. Knight**, K. Anderton, M. Eaton, L.J. Murray

9:30 INOR 1259. Diosmium carbonyl complexes containing multiple ligands derived from ferrocene. **G.L. Powell**

9:50 INOR 1260. Structural elucidation of chemical compounds in reaction conditions that preclude standard characterization techniques. **J. Fehrs**, C.H. Hendon

10:10 Intermission.

10:20 INOR 1261. Bulky β-diketonate ligands and implications for catalysis. **M.P. Marshak**

10:40 INOR 1262. Steps towards the elucidation of the electronic structure of a family of open-shell trinuclear iron clusters. **J. Teesdale**, T. Betley

11:00 INOR 1263. Exploring cooperative redox chemistry using dipyrrin pacman complexes. **E.J. Johnson**, C. Kleinlein, T. Betley

11:20 INOR 1264. Copper(I) and silver(I) complexes with unsaturated N-heterocyclic chalcogenones. **A. Allen**, D. Rabinovich

Section F
Ernest N. Morial Convention Center
Room 354

Environmental & Energy-Related Inorganic Chemistry

S.A. Koch, *Organizer*
J.D. Blakemore, M. Nippe, *Presiding*

8:00 INOR 1265. Modulating electrocatalytic CO_2 reduction via secondary coordination sphere functional groups. S. Sung, J. Meeder, **M. Nippe**

8:20 INOR 1266. Controlled synthesis of earth-abundant tin sulfides Sn_xS_y thin films for photoelectrochemical water splitting. **Y. Liu**, L. Zhang, H. Zhu

8:40 INOR 1267. Bipolar phthalocyanine-based electrolyte for symmetric redox flow batteries. **C. Hunt**, G. Menard

9:00 INOR 1268. Photolytic conversion of light alkanes to alkyl esters by iodine oxides and chloride salts in non-superacidic media. **N. Schwartz**, S.E. Kalman, N. Boaz, J.M. Goldberg, R. Fu, R.J. Nielsen, W.A. Goddard, J.T. Groves, T.B. Gunnoe

9:20 INOR 1269. Carbon dioxide-expanded liquids as media for electrochemistry and catalysis. **J.D. Blakemore**, T. Kerr, C. Shaughnessy, D.J. Sconyers, B. Subramaniam, K.C. Leonard

9:40 INOR 1270. Electrocatalytic reduction of nitrate in water by a highly-fluorinated Cu(II) precatalyst. **J.K. Elinburg**, S. Hannigan, L.H. Doerrer

10:00 INOR 1271. Identification of high ZT thermoelectrics from complex oxide screening. **A. Ganose**, W. Leung, A. Jackson, R. Palgrave, D. Scanlon

10:20 Intermission.

10:40 INOR 1272. Withdrawn

11:00 INOR 1273. Coordination sphere effects on the activity and selectivity of electrochemical CO_2 reduction by a polymer-encapsulated cobalt complex. **Y. Liu**, C.C. McCrory

11:20 INOR 1274. Causes and cures of the photodecomposition of manganese tricarbonyl complexes. **W.C. Henke**, C.J. Otolski, W.N. Moore, K.V. Prather, C.G. Elles, J.D. Blakemore

11:40 INOR 1275. Total utilization of biomass, lignin and carbohydrate: Using earth abundant nickel catalyst. **H. Luo**

12:00 INOR 1276. Palladium N-heterocyclic carbene based CCC-NHC pincer complexes: Air and water stable organometallic emitters. **G.M. Lang**, J. Denny, S. Autry, V. Dixit, N. Hammer, C.E. Webster, T.K. Hollis

Section G
Ernest N. Morial Convention Center
Room 210

Inorganic Catalysts

S.A. Koch, *Organizer*
T. Hamann, D. Powers, *Presiding*

8:30 INOR 1277. Mechanistic insights into the aerobic copper catalyzed decarboxylative thiolation of benzoic acids. **K. Green**, J.M. Hoover

8:50 INOR 1278. Copper cryptand complexes as catalysts for CuAAC click reactions and their prospects for in vivo applications. **T. Tran**

9:10 INOR 1279. Iodine redox catalysts for selective O_2 utilization. **D. Powers**

9:30 INOR 1280. Electrocatalytic reduction of carbon dioxide by finely tuned molecular catalysts. **S. Sung**, D. Kumar, M. Gil-Sepulcre, M. Nippe

9:50 INOR 1281. The influence of ligand environment on the deoxydehydration of polyols by early-metal oxo-complexes. **S.M. Kilyanek**, R. Tran

10:10 Intermission.

10:25 INOR 1282. Understanding the fast rates of open butterfly [2Fe-2S] cluster-based catalysts for the hydrogen-evolving reaction (HER). **K. Clary**, H. Petersen, D.H. Evans, R.S. Glass, D.L. Lichtenberger

10:45 INOR 1283. Formic acid oxidation by surface attached $Ni(P_2N_2)_2$ complexes. **F.M. Brunner**, C.P. Kubiak

11:05 INOR 1284. A molecular palladium catalyst immobilized on heterogeneous metal oxide supports for the hydrodeoxygenation of model lignin monomers. **N.A. DeLucia**, A.K. Vannucci

11:25 INOR 1285. Withdrawn.

11:45 INOR 1286. Fabrication of magnetically retrievable metal nanocatalysts for organic transformations. **R.K. Sharma**

12:05 INOR 1287. Withdrawn

Section H
Ernest N. Morial Convention Center
Room 211

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*
M. Mazzanti, J.D. Rinehart, *Presiding*

8:30 INOR 1288. Generating robust erbium(III) anisotropy without full coordinative saturation for scalable molecule-based magnetic materials. **J.D. Rinehart**, J. Hilgar, M.G. Bernbeck, B. Flores

8:50 INOR 1289. Stabilization of neptunyl crown ether complexes: Characterization by spectroscopic and diffraction approaches. **T. Forbes**

9:10 Intermission.

9:20 INOR 1290. New carbocylic uranium compounds and their unusual reactivity. **K. Erickson**, J.L. Kiplinger

9:40 INOR 1291. Synthesis and reactivity of complexes of f elements supported by siloxide ligands. **M. Mazzanti**

10:00 INOR 1292. Synthesis, characterization and reactivity of U(IV) and U(III) imido and amido complexes with bulky terphenyl substituents. **J.M. Boncella**, B. Billow, A.L. Odom, C. Moktarzadeh

10:20 Intermission.

10:30 INOR 1293. Heterometallic single-molecule magnets: Synthetic challenges and solutions. C. Burns, B. Wilkins, C.M. Dickie, T. Latendresse, **M. Nippe**

10:50 INOR 1294. Synthesis of mixed tris(imido) uranium complexes. **K.E. Gettys**, N. Anderson, M. Zeller, S.C. Bart

11:10 INOR 1295. New bond forming events using organometallic actinide chemistry. **J.K. Pagano**, J. Xie, K. Erickson, D.E. Morris, B. Scott, R. Wu, M. Sykora, P. Yang, R. Waterman, L. Gagliardi, J.L. Kiplinger

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Organometallic Chemistry: New Ligand Platforms

N.S. Radu, *Organizer*
E.T. Papish, *Presiding*

8:30 INOR 1296. Development of new phosphaalkene-pyridine ligands, their coordination chemistry, and use as a noninnocent platform for "waste-free" catalytic processes. **M.L. Nakashige**, M. Cain, A.L. Rheingold

8:50 INOR 1297. Carbon dioxide reduction with transition metals and proton responsive pyridinol based pincer ligands. **E.T. Papish**, S. Das, D.B. Burks, C. Boudreaux, N. Liyanage, S.B. Davis, R.W. Lamb, V. Dixit, F. Qu, C.E. Webster, J.H. Delcamp

9:10 INOR 1298. Synthesis and characterization of "nucleo-pincers" and their transition metal complexes. **S. Gunther**, A.J. Kosanovich, Y. Cao, N. Bhuvanesh, O. Ozerov

9:30 INOR 1299. Robust ruthenium(II) CNC-pincer catalysts selectively reduce carbon dioxide. **C. Boudreaux**, N.

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Liyanage, S. Das, H. Shirley, S. Siek, D. Gerlach, F. Qu, J.H. Delcamp, E.T. Papish

9:50 INOR 1300. New synthetic route to acridone, and acridine-based PNP ligands for low-coordinate late first- and second-row transition metal complexes. **K. Omolo**, J.P. Sadighi

10:10 INOR 1301. Facile dearomatization and metal-ligand cooperation in an unfunctionalized PCP-pincer. **A.J. Kosanovich**, C.H. Komatsu, O. Ozerov

10:30 INOR 1302. Use of a protic bis-(N-heterocyclic carbene)phosphine ligand to explore metal-ligand cooperativity for CO_2 reduction and as a scaffold for bimetallic complexes. **M. Johnson**, S.E. Flowers, B.M. Cossairt

10:50 INOR 1303. Tridentate phosphine ligands bearing aza-crown ether lariats: Applications to Pd and Mo coordination chemistry. **L. Pap**, N. Arulsamy, E.B. Hulley

11:10 INOR 1304. Efficient synthesis of imidoylamidines: The trapping and confirmation of an imidoylamide intermediate. **C.R. Guifarro**, E.V. Rybak-Akimova

Section J
Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N.S. Radu, *Organizer*
B. Captain, U.R. Pokharel, *Presiding*

8:30 INOR 1305. Synthetic methodologies for ferrocene-fused acenes. **U.R. Pokharel**, J. Bergeron, D. Daigle, J.P. Selegue

8:50 INOR 1306. Development of electronic unsaturation in transition metal cluster complexes: Addition of Pt(IPr) groupings as sterically demanding ligands. **V. Zollo**

9:10 INOR 1307. Influence of the isocyanide and Tm ligands on the reductive coupling of $[Tm^{R'}Fe(CNR)_3]OTf$. **O. Mitevski**, A.S. Gowda, A. Baur, J.M. Hoover

9:30 INOR 1308. N_2O binding on $RCo(CNR)_3$ and *O*-atom transfer reactions. **C. Chan**, J.S. Figueroa

9:50 Intermission.

9:55 INOR 1309. Synthesis of formazanate complexes with third row transition metals and analysis of their spectroscopic and electrochemical properties. **E. Kabir**, T. Teets

10:15 INOR 1310. Further developments in synthesis from $[M(S_2C_2Ph_2)_2]$ (M = Ni, Pd, Pt) by direct ligand substitution. **A. Obanda**, K. Martinez, R.H. Schmehl, I.V. Rubtsov, J.T. Mague, J.P. Donahue

10:35 INOR 1311. Small molecule activation by platinum complexes containing bulky tin groups. **B. Captain**, A. Koppaka, M. Gamage

10:55 INOR 1312. Synthesis, structures and properties of copper complexes with diaminobis(thiolato) ligands. **B. Wang**, S.J. Ferrara, S. Sproules, R. Pascal, J.T. Mague, J.P. Donahue

11:15 INOR 1313. Group 10 dithiolene compounds with an open-ended 1,2,4,5-Tetrakis(diphenylphosphino) benzene ligand: Synthesis, structure, properties. **M. Pratheepkumar**, K. Arumugam, J.T. Mague, **J.P. Donahue**

Section K
Ernest N. Morial Convention Center
Room 335

Chemistry of Materials: Nanomaterials

C.G. Lugmair, *Organizer*
M. Devadas, *Presiding*

8:00 INOR 1314. Combinatorial synthesis of multimetallic nanoparticles. **P. Chen**, J. Hedrick, C.A. Mirkin

8:20 INOR 1315. Host-guest design to access the lead halide perovskites nanocrystals under strong confinement using metal organic frameworks as a matrix. **L. Protesescu**, M. Dinca

8:40 INOR 1316. Photo–inks based on porphyrins and diarylethenes (DAEs). A. Galanti, T. Biellmann, J. Wytko, J. Boixel, V. Guerchais, P. Samori, **J. Weiss**

9:00 INOR 1317. Introducing room temperature liquid metals as a reaction solvent for the synthesis of atomically thin 2D metal oxides. **T. Daeneke**, A. Zavabeti, R.B. Kaner, K. Kalantar-zadeh

9:20 INOR 1318. Investigating inter-particle exchanges and crystallographic changes in gold nanoclusters. **C. Hosier**, C. Ackerson

9:40 Intermission.

9:55 INOR 1319. Synthesis of first row transition metals nanoparticles for aerosol deposition. **L.J. Treadwell**, T.J. Boyle, A.W. Cook, D. Perales, D. Woodard, N.S. Bell

10:15 INOR 1320. Controlled growth of Mn_{12} single-molecule magnet polymers and oligomers. M. Shmunes, E.R. Williams, S.M. Stone, A.M. Mowson, G. Christou, T.M. Pekarek, **C. Lampropoulos**

10:35 INOR 1321. Au(I) precursors for electron beam induced deposition. **W.G. Carden**, J. Pedziwiatr, K.A. Abboud, L. McElwee-White

10:55 INOR 1322. Magic numbered gold clusters–optical and electrochemical properties. **M. Devadas**, A. Meola, B. Hutson, N. Hondrogiannis, K. Reber

11:15 INOR 1323. Pulsed microwave energy: A kinetic control approach to highly branched nickel multipod nanostructures. **P. Vakil**, B. Ashley, D. Hardy, G.F. Strouse

11:35 INOR 1324. Surfactant-free shape control of gold nanoparticles enabled by unified theoretical framework of nanocrystal synthesis. **C.M. Drain**, M. Wall, M. Kircher

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde
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THURSDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 345

Chemistry of Materials: Metal Organic Frameworks

C.G. Lugmair, *Organizer*
C.H. Hendon, *Presiding*

1:30 INOR 1325. Development of a computational method for simple DFT calculation of pore volume and surface area of porous materials. **C.H. Hendon**, K. Butler, T.Z. Crawford

1:50 INOR 1326. Withdrawn.

2:10 INOR 1327. Tubes vs sheets: A mechanistic investigation of MOF dimensionality. **K.M. Vailonis**, U. Shrestha, M.D. Dadmun, D.M. Jenkins

2:30 INOR 1328. Biocompatible near-infrared MOF fluorophores for bio-imaging applications. **D.F. Sava Gallis**, L.S. Rohwer, K.S. Butler, T.S. Luk

2:50 INOR 1329. Withdrawn.

3:10 Intermission.

3:25 INOR 1330. Mesoporous MOFs for DNA and protein Inclusion. **H. Deng**

3:45 INOR 1331. Lanthanide metal-organic frameworks for proton conduction. **M. Fairley**, L. Qin, Z. Zheng

4:05 INOR 1332. Luminescent conductive metal-organic frameworks. **G. Skorupskii**, K. Williams, R.W. Day, C. Perkinson, M. Cotlet, M. Baldo, W.A. Tisdale, M. Dinca

4:25 INOR 1333. Electronic structure of electrically conductive metal organic frameworks. **J. Fehrs**, C.H. Hendon

4:45 INOR 1334. Boosting transport distances for molecular excitons within photo-excited metal–organic framework films. **S. Goswami**, M. Chen, M.R. Wasielewski, O.K. Farha, J.T. Hupp

Section B
Ernest N. Morial Convention Center
Room 344

Coordination Chemistry: Synthesis & Characterization

A. Larsen, *Organizer*
C. Martin, N.C. Tomson, *Presiding*

1:30 INOR 1335. Exploiting the Lewis acidity of boroles to access boron-containing heterocycles. S. Yruegas, V. Adiraju, **C. Martin**

1:50 INOR 1336. Structural and spectroscopic characterization of five-coordinate iron and cobalt bis(dithiolene)-phosphine complexes. **P. Chandrasekaran**, L. Mootha, D. Williams

2:10 INOR 1337. Coordination chemistry of extended pyridyl-acetylacetonate ligands. **C.A. Gunawardana**, A. Sinha, V. Day, C.B. Aakeroy

2:30 INOR 1338. Oxidative reactivity of a rhenium nitride complex. **G.P. Connor**, P.L. Holland, J.M. Mayer

2:50 Intermission.

3:00 INOR 1339. Synthesis and structure of octahedral cobalt clusters. **R.A. Musgrave**, A.R. Fout, R. Hernandez Sanchez, T. Betley

3:20 INOR 1340. Synthesis, characterization, and reactivity of thermally stable cupric superoxides. S. McCollom, A.B. Weberg, P.J. Carroll, **N.C. Tomson**

3:40 INOR 1341. Experimental and computational studies of trans-Rh_2 compounds: Improving the photochemistry by manipulating the configurational isomerism. **A. Millet**, C. Xue, C. Turro, K.R. Dunbar

4:00 INOR 1342. Synthesis, characterization, and reactivity of luminescent CuCl complexes with triaminoborane-bridged diphosphines. **C.M. Donahue**, K. Lee, B.A. Massman, S.R. Daly

4:20 INOR 1343. Withdrawn.

Section C

Ernest N. Morial Convention Center
Room 343

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N.S. Radu, *Organizer*
J.P. Donahue, *Presiding*

1:30 INOR 1344. Homoleptic platinum azo-iminate complexes via hydrogenative cleavage of formazans. **G. Mu**, T.S. Teets

1:50 INOR 1345. The 4-electron reduction of benzo[c]cinnoline by a trimetallic Ni_2Ti complex. **P. Dunn**, I. Tonks

2:10 INOR 1346. Revisiting the cluster-surface analogy: Surface-like behavior in strong field iron clusters. **M.J. Drance**, J.S. Figueroa

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2:30 INOR 1347. Structure and reactivity of mono-anionic rhodium and iridium tris-isocyanides. **M.L. Neville**, J.S. Figueroa

2:50 INOR 1348. Investigations of a reactive open shell trigold(I) carbide and its adducts. **N.T. Daugherty**, J.P. Sadighi, J. Bacsa

3:10 INOR 1349. Withdrawn.

3:30 INOR 1350. Isolation and characterization of in-situ species formed in iron-catalyzed cross-coupling reactions with aryl nucleophiles. **S. Carpenter**, M.L. Neidig

3:50 INOR 1351. Synthesis and characterization of high-spin iron carbene complexes. **A. Wrobel**, T. Betley

Section D
Ernest N. Morial Convention Center
Room 352

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S.A. Koch, *Organizer*
W.M. Ames, H.R. Lucas, *Presiding*

1:30 INOR 1352. New chemical tools for studying cellular iron homeostasis. **A. Fikes**, E.L. Que

1:50 INOR 1353. Biological on/off switch for bacterial biofilm formation in *Agrobacterium vitis*. **D. Williams**, N.M. Nesbitt, E.M. Boon

2:10 INOR 1354. Formation of benzothiazoles from 2-mercaptoaniline and O_2-dependent oxidation of primary alcohols by thiol dioxygenase enzymes. **S. Sardar**, W.P. Morrow, F.W. Foss, B.S. Pierce

2:30 INOR 1355. Mutations on the superoxide reductase: A theoretical study of the 2nd coordination sphere and formation of an oxo-iron intermediate. **R. David**, H. Jamet, V. Nivière, Y. Moreau, A. Milet

2:50 INOR 1356. Reactivity of diiron clusters containing sulfide and hydride bridges. **D. Singh**, B. Knight, L.J. Murray

3:10 INOR 1357. Investigating unique *J*-values for $Mn^{III}Mn^{III}$ and $Mn^{III}Mn^{IV}$ dimers containing a single unsupported μ-oxo bridge with BS-DFT. **W.M. Ames**

3:30 Intermission.

3:45 INOR 1358. Triplet, high-spin, linear $\{Fe(NO)\}^8$: Redox feature of a stable diiron trinitrosyl complex. **P. Ghosh**, S. Ding, M. Quiroz, C. Hsieh, M.B. Hall, M.Y. Darensbourg

4:05 INOR 1359. Nickel and cobalt macrocycles for oxidative transformations. **H.R. Lucas**

4:25 INOR 1360. Molecular modelling on the driving force the acylation of β -lactam antibiotics. **C.U. Ibeji**

Section E
Ernest N. Morial Convention Center
Room 353

Chemistry of Materials: Nanomaterials

C.G. Lugmair, *Organizer*
A.L. Eckermann, *Presiding*

1:30 INOR 1361. Europium-doped cerium oxide nanomaterials: Synthesis and exposure to l-dopa and eumelanin. **A. D'Achille**, J.L. Coffer

1:50 INOR 1362. Gold nanoparticles stabilized by organic-inorganic hybrid polyoxometalates: Synthesis, surface studies and catalytic applications. **M. Martin Gandul**, G. Newton

2:10 INOR 1363. Thermal decomposition of Prussian blue analogue as precursors for magnetic nanoparticles. **D.A. Hardy**, G.F. Strouse

2:30 INOR 1364. Synthesis of 2D metal borides derived from ternary MAB phases. **L. Alameda**, R.E. Schaak

2:50 INOR 1365. Synthesis and leaching of strontium-doped hydroxyapatite. **A.L. Eckermann**, A. Washburn, K. Libson

3:10 INOR 1366. Minerals to materials: Bulk synthesis of aqueous aluminum clusters and their use as precursors for metal oxide thin films. **B. Fulton**

3:30 Intermission.

3:45 INOR 1367. Carbon nanorods for water expulsion at high humidity. **J. Kothandaraman**, S.K. Nune, D.J. Heldebrant, M.J. Olszta, D. Lao, K. Stoerzinger, Y. Shin, X. Yu

4:05 INOR 1368. Molybdenum promoted mesoporous Co_3O_4: Study of acid-base switchable surface chemistry. **C. Weerakkody**, S.L. Suib

4:25 INOR 1369. Temperature dependant stabilites of various isomers of C32 endohedral metallofullerenes. **T.J. Fuhrer**, S. Church, J. Coello

4:45 INOR 1370. Purification of metallic nanowires and their uses in low density aerogels. **Y. Han**, F. Qian

5:05 INOR 1371. Van der Waals assembly of two-dimensional fullerene thin films. **K. Lee**, B. Choi, I. Jen-La Plante, C. Goulbourne, X. Zhu, X. Roy

5:25 INOR 1372. Exploring synthetic pathways to pluronics-derived mesoporous nitrides with *in situ* SAXS/WAXS. **P. Beaucage**, S.M. Gruner, U.B. Wiesner

Section F
Ernest N. Morial Convention Center
Room 354

Chemistry of Materials: Synthesis & Properties

C.G. Lugmair, *Organizer*
F. Fallah Tafti, T.E. Stevens, *Presiding*

1:30 INOR 1373. Tuning superconductivity and magnetism in $[Li_{1-x}Fe_xOH]FeS$ by controlling the hydrothermal synthesis conditions. **F. Fallah Tafti**, E. McDonnell

1:50 INOR 1374. Plasmonic excitations in strained $Sr_{1-x}Nb_{1-y}O_{3+}$β nanoparticles. **T. Ofoegbuna**, W. Shelton, J.A. Dorman

2:10 INOR 1375. Near-infrared aza-BODIPY fluorescence probes for selective Cu^{2+} detection and their potential in living cell imaging. **N. Wanichacheva**, Y. Tachapermpon, P. Praikaew, S. Thavornpradit, A. Charoenpanich, J. Sirirak, K. Burgess

2:30 INOR 1376. Chemically tunable photoluminescence in Si_2Te_3nanoplates through doping and intercalation. **M. Wang**, B. Wang, K.J. Koski

2:50 Intermission.

3:05 INOR 1377. Synthesis of a magnetically frustrated organometallic ferrous oxide cluster from partial oxidation. **Z.H. Hecht**, J. Kephart, N. Arulsamy, B. Livesay, M.P. Shores, C.V. Popescu, E.B. Hulley

3:25 INOR 1378. Synthesis of β'-Fe_4N, a new soft magnetic material for inductors and transformers. **T.E. Stevens**, C.J. Pearce, S. Atcitty, T.C. Monson

3:45 INOR 1379. Using different synthetic conditions to achieve maximum dye loading of Brooker's merocyanine within zeolite L channels. **J.S. Holt**, L. Engerer, T. Dabertin, B. Henning, S. Mattis, K. Weber

4:05 INOR 1380. Kinetic control of ZnS and ZnSe nanocrystal syntheses. **E. Bennett**, L. Hamachi, H. Yang, B. Abecassis, J. De Roo, M. Greenberg, J.S. Owen

Section G
Ernest N. Morial Convention Center
Room 210

Coordination Chemistry: Characterization & Applications

A. Larsen, *Organizer*
K.L. Mulfort, M. Zdilla, *Presiding*

1:30 INOR 1381. Vectorial charge transfer from heteroleptic Cu(I)diimine complexes. **K.L. Mulfort**, L. Kohler, D. Hayes, R.G. Hadt, L.X. Chen

1:50 INOR 1382. Pyrazole-based ligands for complexation, extraction and recovery of Hg(II) from nuclear waste. **S. Kandel**, K. Chambers, L. Mathivathanan, R.G. Raptis

2:10 INOR 1383. Aminotriphenolate complexes for catalysis and enantioselective molecular recognition. C. Zonta, A.W. Kleij, **G. Licini**

2:30 INOR 1384. Synthesis and elucidation of novel phosphonate-based biocompatible coordination polymers with enhanced dissolution properties. **G. Quinones Velez**, V. López-Mejías

2:50 INOR 1385. Breaching the "CHNO ceiling" in energetic materials by the inclusion of redox-frustrated inorganic elements.. **M. Zdilla**, O. O'Sullivan

3:10 INOR 1386. Tunable dimetal tetraguanidinate paddlewheel complexes with unprecedented electron donor abilities. **M. Humphries**, B.R. Smith, E. Wusterbarth, J.T. Njardarson, D.L. Lichtenberger

3:30 INOR 1387. Inorganic-organic hybrid material for the cyanide sensing using Co(II)-bis-terpyridine type coordination complexes. **I. Bhowmick**, C. Collins, D.J. Boston

3:50 Intermission.

4:00 INOR 1388. Synthesis, characterization, and reactivity studies of a zirconium-cobalt bis(phosphinoamide) complex. **K.M. Gramigna**, C.M. Thomas

Section H
Ernest N. Morial Convention Center
Room 337

Nanoscience

B.G. Trewyn, *Organizer*
J.E. Johns, *Presiding*

1:30 INOR 1389. Cancer nanotherapy promoted by a nuclear targeting molecular capsule. **Y. Fang**, H. Zhou

1:50 INOR 1390. Ultrastable metal nanoparticles studied for the development of biomedical applications, nanomedicine and water purification. **E. Rauwel**, P. Rauwel, S. Küünal, O. Volobujeva, A. Ivask, D. Wragg

2:10 INOR 1391. Controlling DNA delivery from gold nanoparticles in human cells, studied via live-cell fluorescence microscopy. **K.J. Carnevale**, G.F. Strouse

2:30 INOR 1392. Nanobioplar electrodeposition in nanoparticle arrays for tunable optical materials. **G. Crouch**, D. Han, S. Fullerton, D. Go, P.W. Bohn

2:50 Intermission.

3:00 INOR 1393. Impact of natural organic ligands structure on the colloidal stability of silver nanoparticles. **K. Afshinnia**, M. Baalousha

3:20 INOR 1394. Oil separation from water under environmentally relevant conditions using polymer-coated iron oxide nanoparticles. **S. Mirshahghassemi**, J. Lead

3:40 INOR 1395. Ultrathin nanowires of Mo_6Te_6 grown by chemical vapor deposition. **J.E. Johns**, Y. Yoo, J. Jeong

4:00 INOR 1396. Structural characterization and sulfide oxidation of V-DTPA immobilized on mesoporous silica. **J.R. Taft**, C.C. Landry

Section I
Ernest N. Morial Convention Center
Rooms 340/341

Chemistry of Materials: Materials for Energy & Catalytic Applications

C.G. Lugmair, *Organizer*
M.P. Campos, *Presiding*

1:30 INOR 1397. Synthetic manipulation of hybrid thermoelectric materials. **K.A. Mazzio**, M. Raja Thulasimani, B. Ryll, D. Kojda, K. Habicht, S. Raoux

1:50 INOR 1398. Bismuth chalcohalides as earth-abundant and non-toxic photovoltaics. **A. Ganose**, K. Butler, A. Walsh, D. Scanlon

2:10 INOR 1399. Structured Si/Co-P photocathodes: Designs for efficient light absorption in earth abundant solar fuels devices. **P. Kempler**, M. Gonzalez, K. Papadantonakis, N.S. Lewis

2:30 INOR 1400. Quantum dot nucleation and the future of LED lighting. **M.P. Campos**, L. Hamachi, M.P. Hendricks, I. Rreza, J. De Roo, J.S. Owen

2:50 Intermission.

3:05 INOR 1401. Sequential series multijunction dye-sensitized solar cells (SSM-DSCs): Concept, optimizations and novel applications. **H. Cheema**, J.H. Delcamp

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3:20 INOR 1402. (Photo)electrocatalytic properties of copper gallium delafossite nanoflakes. **Y. Mao**, S. Mohan

3:40 INOR 1403. Ultrathin metal/semiconductor nanosheets for photocatalytic oxidation of alcohols and H_2 evolution. **G. Han**, Y. Sun

4:00 INOR 1404. Photocatalytic degradation of low concentration toluene by atomically platinum dispersed nanoporous TiO_2 film with exposed {001} facets. **H. Zheng**, T. Xu, P. Zhang

Section J
Ernest N. Morial Convention Center
Room 212

Organometallic Chemistry: Catalysis-Late Transition Metals

N.S. Radu, *Organizer*
B.P. Carrow, E.A. Ison, *Presiding*

1:30 INOR 1405. Synthesis and reactivity studies of a [Cp*Rh] monohydride. **E. Boyd**, K.V. Prather, D. Lionetti, J.D. Blakemore

1:50 INOR 1406. Mechanism of the Tishchenko reaction catalyzed by an octahedral d^6-rhodium dihydride catalyst. **J. Mallah**, **F. Hasanayn**

2:10 INOR 1407. Azaphosphatriptycene in rhodium-catalyzed hydroformylation. **Y. Cao**, J. Napoline, J. Bacsa, J.P. Sadighi

2:30 INOR 1408. Pentamethylcyclopentadiene as a ligand in rhodium-catalyzed hydrogen evolution. **Y. Peng**, D. Lionetti, J.D. Blakemore

2:50 INOR 1409. Insights into catalytically active rhodium complexes. **D. Selent**, C. Kubis, A. Boerner, W. Baumann, K. Neymeyr, M. Sawall, H. Schroeder

3:10 INOR 1410. Rhodium complexes ligated by an unconjugated bipyridine analogue: Electronic properties and effects on H_2 evolution reactivity. **D. Lionetti**, V. Day, J.D. Blakemore

3:30 INOR 1411. Nickel dipyrrin imides capable of C–H bond amination. **Y. Dong**, T. Betley

3:50 INOR 1412. Through-space ligand effects on reaction rate and selectivity in gold(acyclic diaminocarbene)-catalyzed organic transformations. A.A. Ruch, J.K. Nguyen, M.C. Ellison, **L.M. Slaughter**

4:10 INOR 1413. Non-covalent interactions in rhenium oxo/nitrido frustrated Lewis pairs. **E.A. Ison**, N.S. Lambic

4:30 INOR 1414. Selective reduction of CO_2: A rational thermodynamic approach to disfavor proton reduction pathways. **D.W. Cunningham**, J.Y. Yang

4:50 INOR 1415. Unstable boronic acid and pinacol ester cross-coupling enabled by an "on-cycle" precatalyst. **B.P. Carrow**

5:10 INOR 1416. Catalytic N-formylation of amines using CO_2 and H_2. **U. Jayarathne**, N. Hazari, W.H. Bernskoetter

Section K
Ernest N. Morial Convention Center
Room 335

Chemistry of Materials: Metal Organic Frameworks

C.G. Lugmair, *Organizer*
T. Gadzikwa, Q. Zhang, *Presiding*

1:30 INOR 1417. Synthesis and characterization of high valence metal phosphonate metal-organic frameworks. **D.B. Barbee**, A.R. Barron

1:50 INOR 1418. Bio-template synthesis of zeolitic imidazolate framework-8 (ZIF-8). **Q. Wang**, H. Qin, H. Zhou

2:10 INOR 1419. Phase-purity and size control of NU-1000. **T. Webber**, S. Bingham, R. Combs, W. Liu, S.P. Desai, C. Lu, D.G. Truhlar, R. Penn

2:30 INOR 1420. Precise control of the pore hydrophilicity enabled by post-synthetic cation exchange in a metal-organic framework. **A.M. Wright**, A.J. Rieth, M. Dinca

2:50 INOR 1421. Synthesis and applications of hierarchically structured metal–organic frameworks. **Y. Yue**, S. Armentrout

3:10 Intermission.

3:25 INOR 1422. Some general considerations made for controlled guest materials formation in the confined environments of metal-organic frameworks. **T. Wang**, S.K. Smoukov, A.K. Cheetham

3:45 INOR 1423. Topological transformation of luminescent metal–organic frameworks. **Q. Zhang**

4:05 INOR 1424. Synthetic strategies for constructing enzyme-inspired metal=organic framework materials. **T. Gadzikwa**, C.S. Satterfield, K.P. Samarakoon, M.C. McCoy

4:25 INOR 1425. *Quo vadis niobium?* Multifaceted coordination behavior of MOF-5. **M.D. Korzynski**, L. Braglia, E. Borfecchia, A. Baldansuren, C.H. Hendon, C. Lamberti, M. Dinca

4:45 INOR 1426. Cross-linking Zr-based metal-organic polyhedra via postsynthetic polymerization. **D. Nam**, J. Huh, J. Lee, J. Kwak, H. Jeong, K. Choi, W. Choe

Celebrating Over Four Decades of Research in Nanomaterials & Commercialization: Symposium in honor of Kenneth Klabunde
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Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

Molecular Processes at Mineral-Water Interfaces: Linking Theory & Experiments

Uranium Incorporation: Sulfate Mineral Geochemistry

Sponsored by GEOC, Cosponsored by ENVR and INOR

Catalytic Conversion of Biomass Derived Molecules to Chemicals & Fuels
Sponsored by CATL, Cosponsored by ENFL, ENVR and INOR

Theoretical & Experimental Studies of Supercritical Fluids in the Subsurface
Sponsored by GEOC, Cosponsored by ENVR and INOR

Control of Zeolite Structure, Composition & Sites for Catalysis
Sponsored by CATL, Cosponsored by INOR

‡*Cooperative Cosponsorship*

MEDI

Division of Medicinal Chemistry

A. Stamford, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Advances in Molecular Recognition of Double-Helical DNA & RNA (see *CARB*, Mon, Tue)

Discovery of Small Molecules Targeting RNA (see *ORGN*, Tue)

Structure-Based Drug Design for GPCRs (see *COMP*, Wed)

SOCIAL EVENTS:

Poster Session & Social Hour, 7:00 PM: Sun, Wed

BUSINESS MEETINGS:

Business Meeting, 5:30 PM: Sun

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

Leveraging Atropisomers in Medicinal Chemistry

M.M. Weiss, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 MEDI 1. Atropisomer axial chirality as a valuable tool in drug discovery. **S. LaPlante**

9:10 MEDI 2. Atropisomerism in macrocyclic factor VIIa inhibitors. **P. Glunz**, N. Wurtz, X. Zhang, L. Mueller, D.L. Cheney, A. Wei, P. Wong, R.R. Wexler, E.S. Priestley

9:45 MEDI 3. Leveraging atropisomerism in the identification of $Na_v1.7$ inhibitors for the treatment of pain. **B.C. Milgram**, M. Chu-Moyer, E.F. DiMauro, H. Gao, A. Guzman-Perez, D. La, I.E. Marx, B. Moyer, A. Boezio, J. Butler, R. Graceffa, C. Kreiman, E. Peterson, B. Sparling, K. Romero, M.M. Weiss

10:20 MEDI 4. Atropisomerism as a means to modulate target selectivity and an inspiration for new chemistry. **J. Gustafson**

10:55 MEDI 5. Optimizing kinase in the development of lorlatinib: The challenge of atropisomerism. **P. Richardson**

11:30 MEDI 6. Twisted road to the discovery of BMS-986142: Using conformationally locked atropisomers to drive potency in a reversible inhibitor of Bruton's tyrosine kinase (BTK). **S.H. Watterson**, G.V. De Lucca, Q. Shi, C.M. Langevine, Q. Liu, D.G. Batt, M. Beaudoin Bertrand, H. Gong, J. Dai, H. Yip, P. Li, D.Z. Sun, D. Wu, C. Wang, Y. Zhang, S.C. Traeger, M. Pattoli, S. Skala, L. Cheng, M.T. Obermeier, R. Vickery, L. Discenza, C. D'Arienzo, K.M. Gillooly, T. Taylor, C. Pulicicchio, K.W. McIntyre, M.A. Galella, A. Tebben, J. Muckelbauer, C. Chang, L. Salter-Cid, J.C. Barrish, P.H. Carter, A. Fura, J.R. Burke, J.A. Tino

Section B
Ernest N. Morial Convention Center
Rooms 252-254

General Orals

A.W. Stamford, *Organizer*
J.R. Allen, *Presiding*

8:30 MEDI 7. Inhaled Janus kinase 1 (JAK1) inhibitors as potential treatments for asthma. **M. Zak**, N. Ray, S. Goodacre, N. Ghilardi, H. Dengler, C. Rinderknecht, A. Johnson, M. Briggs, B. McKenzie, D. Brown, J. Kenny

8:50 MEDI 8. Discovery of LAS194046, a potent pan-JAK inhibitor for the inhaled treatment of respiratory diseases. **J. Bach**

9:10 MEDI 9. Design of KDM4C inhibitors with antiproliferative effects in cancer models. **Y. Chen**

9:30 MEDI 10. Small molecules as frontline therapy for immune oncology: Experience from ubiquitin pathway targets. **J. Wu**, S. Kumar, F. Wang, I. Sokirniy, M. Mattern, J. Weinstock

9:50 MEDI 11. Small molecule screening approaches for inhibition of Ubc9 and the sumoylation pathway. **K. Zlotkowski**, W.M. Hewitt, G. Lountos, S. Dahlhauser, L. Saunders, R. Sinniah, D. Needle, J. Tropea, B. Ma, P. Yan, H. Bokesch, M.L. Peach, M.C. Nicklaus, J.J. Barchi, J. McMahon, R. Nussinov, D. Waugh, K. Gustafson, J. Schneekloth

10:10 MEDI 12. Evaluation of triazolopyrimidine microtubule-stabilizing small molecules as potential candidates for the treatment of Alzheimer's disease and related tauopathies. **C. Ballatore**, Y. Yao, K. Oukoloff, A. Cornec, M. James, J. Trojanowski, V. Lee, A.B. Smith, K. Brunden

10:30 MEDI 13. Synthesis and characterization of a highly potent series of substituted N-(indanyl)piperidine-4-carboxamides as positive allosteric modulators of the M_5 muscarinic acetylcholine receptor. **A. Bender**, K.D. Nance, H.P. Cho, T.M. Bridges, P.M. Sexton, A. Christopoulos, P.J. Conn, C.W. Lindsley

10:50 MEDI 14. Discovery and design of novel selective kappa opioid antagonists. **M. Green**, N. Kablaoui, R. Danica, C.M. Stiff, B. Brian, K.J. Coffman, M.A. Brodney, P.R. Verhoest

11:10 MEDI 15. Macrocyclic peptides as novel LSD1 inhibitors and their biological evaluation. **I.R. Kumarasinghe**, P.M. Woster

11:30 MEDI 16. Design and synthesis of lysine-targeted covalent inhibitors of HSP72. **J. Pettinger**, Y. Le Bihan, M. Powers, M. Widya, R. van Montfort, K. Jones, M. Cheeseman

11:50 MEDI 17. Indole-2-carboxamides (I2Cs) targets mycolic acid transport and offer a potential treatment for *Mycobacterium abscessus* infections. **O. Onajole**, J. Stec, C. Dupont, A. Viljoen, M. Richard, T. Chaira, S. Lun, W. Bishai, S. Raj, D. Ordway, A.P. Kozikowski, L. Kremer

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

General Orals

A.W. Stamford, Organizer, Presiding

1:30 MEDI 18. Discovery of a potent and efficacious Mcl-1 inhibitor featuring an β-hydroxy phenylacetic acid pharmacophore. **G. Rescourio**, S.P. Brown

1:55 MEDI 19. Discovery of SAM competitive, brain-restricted PRMT5 inhibitors with potent antitumor activity. **J.H. Tatlock**, J. Billitti, J.F. Braganza, A. Brooun, Y. Deng, B. Hirakawa, K. Jensen-Pergakes, R. Kumpf, W. Liu, K. Maegley, I.J. McAlpine, M. McTigue, R. Patman, E. Rui, S.A. Scales, M.B. Tran-Dube, F. Wang, Z. Wang, S. Yamazaki, T. Zhang, M. Wythes

2:20 MEDI 20. Optimization of S1P1 partial agonists leading to the identification of BMS-986166. **A.J. Dyckman**, J.L. Gilmore, M. Yang, T. Dhar, D. Marcoux, Z. Xiao, H. Xiao, L. Li, A. Mathur, J. Xie, K. McIntyre, R. Thomas, T. Taylor, X. Yang, L. Lehman-McKeeman, H. Shi, P.C. Levesque, H. Sun, A.M. Marino, Z. Yang, G. Cornelius, C. D'Arienzo, D. Shen, M. Cvijic, B.M. Warrack, L. Salter-Cid, L. Lombardo, J.E. Macor, P.H. Carter

2:45 MEDI 21. Inhibition of glutaminyl cyclase as a new concept for the treatment of Alzheimer's disease: PQ912, the first-in-class QC-inhibitor in clinical development for AD. **U. Heiser**, T. Hoffmann, A. Meyer, R. Sommer, D. Ramsbeck, M. Kleinschmidt, H.U. Demuth, K. Glund, I. Lues

3:10 MEDI 22. Discovery of clinical candidate TAK-915, a highly potent, selective, and brain-penetrating phosphodiesterase 2A inhibitor for the treatment of cognitive disorders. **S. Mikami**, S. Nakamura, T. Ashizawa, I. Nomura, M. Kawasaki, S. Sasaki, H. Oki, H. Kokubo, I.D. Hoffman, H. Zou, N. Uchiyama, K. Nakashima, N. Kamiguchi, H. Imada, N. Suzuki, H. Iwashita, T. Taniguchi

3:35 MEDI 23. Discovery of potent and orally bioavailable macrocyclic peptide-peptoid hybrid CXCR7 modulators. **M. Boehm**

4:00 MEDI 24. Novel RORβ inverse agonists: From GDC-0022 to a novel pyridazine-based series. **J.J. Crawford**

4:25 MEDI 25. Discovery and development of novel small molecule modulators of TNF alpha signalling. **D. Brookings**, R.P. Alexander, T. Arakaki, J. Bentley, T. Bourne, J.A. Brown, A. Burgin, M. Calmiano, B. Carrington, M. Deligney, D. Fox III, A. Foley, H.T. Horsley, J. Heer, J. Henshall, M. Hutchings, V. Jackson, C. Johnstone, J. Kennedy, L. King, B. Kroeplien, A. Lawson, F. Lecomte, J. Madden, K. Menochet, M. Merriman, T. Norman, J. O'Connell, A. Payne, J. Porter, J. Quincey, S. Rapecki, M.D. Selby, A. Vugler, G. Watt, S. Wright, Z. Zhu

4:50 MEDI 26. Discovery of a novel series of small molecule modulators of TNF alpha binding and signalling through a novel mechanism of action. **T. Norman**, F. Lecomte, J. Kennedy, B. Carrington, J. Porter, J. O'Connell, A. Lawson, R. Davis, S. Rapecki, B. Kroeplien, A. Burgin, T. Arakaki

Section B
Ernest N. Morial Convention Center
Rooms 252-254

Medicinal Chemists' Toolbox Series: Dipole & Charge in Drug Design

N.A. Meanwell, P.M. Scola, K. Yeung, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 MEDI 27. Deeper understanding of molecular recognition through modern computational techniques. **C.D. Sherrill**, R.M. Parrish, D. Sitkoff, D.L. Cheney

2:10 MEDI 28. Electrostatic basis of anomalous SAR and molecular properties: Tactical lessons in drug design. **D.L. Cheney**, D. Sitkoff, X. Zhu, M. Dhar, B.W. Bakr, C.D. Sherrill

2:45 MEDI 29. Fluorine multipolar interaction: how much does it contribute to binding free energy? **L. Xing**

3:20 MEDI 30. Understanding stacking interactions of heterocyclic drug fragments. **S.E. Wheeler**, A.N. Bootsma, A.C. Doney

3:55 MEDI 31. Polar protein-ligand interactions: Statistical significance and use in structure-guided drug design. **B. Kuhn**

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall E

General Posters

A.W. Stamford, *Organizer*

7:00–9:00

MEDI 32. Discovery of a highly selective BTK inhibitor Tirabrutinib(ONO/GS-4059) for B-cell lymphoma and inflammatory diseases. **S. Yamamoto**, R. Suzuki, A. Hiramatsu, H. Kijima, T. Watanabe, H. Egashira, S. Takai, M. Terakado, S. Ogawa, M. Ima, T. Nishiyama, I. Doi, M. Kurono, R. Omi, K. Kayasuga, S. Kusuda, A. Imagawa, H. Habashita, T. Seko, K. Moriarty, Z. Konteatis, K. Moffett, Y. Lee, W. Chao

MEDI 33. Photoaffinity labeling approach towards binding site identification of chroman-4- one based sirtuin 2 inhibitors. **T. Seifert**, M. Malo, J. Lengqvist, C. Sihlbom, E.M. Jarho, K. Luthman

MEDI 34. Discovery of a novel kinase inhibitor ON 150030, a type 1 inhibitor for relapsed and refractory AML. **M. Reddy**, H. Ghaffari, B. Akula, S.C. Cosenza, M.R. Mallireddigari, V. Dandu, P. Reddy

MEDI 35. Discovery of pyrrolo[1,2-b] pyridazine-3-carboxamides as potent JAK1/3 inhibitors with selectivity against ROCK family kinases. **S. Spergel**, M.E. Mertzman, S. Lin, G. Brown, J. Kempson, J. Guo, S.M. Stachura, J.S. Lippy, R.F. Zhang, S. Pitt, A. Fura, V. Tang, J.S. Tokarski, J. Sack, J. Khan, J. Li, J. Hennan, P.C. Levesque, P.H. Carter, J.C. Barrish, L. Salter-Cid, G.L. Schieven, S. Wrobleski, W.J. Pitts

MEDI 36. Discovery and structure-activity relationship of pyrrolo[2,1-f] [1,2,4]triazines as inhibitors of phosphatidylinositol 3-kinase β (PI3Kβ) for the treatment of immunological disorders. **Q. Shi**, D. Marcoux, Q. Liu, D.G. Batt, L. Cornelius, A.S. Srivastava, R.J. Cherney, L. Qin, Z. Ruan, J. Neels, R.S. Bhide, L. Li, M. Beaudoin Bertrand, H. Gong, S.H. Watterson, J. Pan, H. Tang, J. Fan, M. Yarde, M. Cvijic, M.T. Obermeier, A. Fura, C.A. Weigelt, M.A. Galella, J. Sack, J. Muckelbauer, K.M. Gillooly, K.W. McIntyre, Q. Ruan, M.A. Poss, J. Hynes, J.E. Macor, P.H. Carter, S. Ruepp, G.L. Schieven, J.A. Tino

MEDI 37. Highly delta selective quinazolinone PI3K inhibitors. **J.A. Treiberg**, J. Chandrasekhar, C. Ip, D. Koditek, E. Lepist, M. McGrath, J. Mwangi, S. Perreault, J. Somoza, B. Steiner, J.H. Therrien, A.G. Villasenor, S. Wise, B. Wong, G. Phillips

MEDI 38. Dual kinase-bromodomain inhibition of Brd4 and p38a using trisubstituted-imidazoles. **A. Divakaran**, S.K. Talluri, A.M. Ayoub, N.K. Mishra, J.C. Widen, J. Zhu, N. Berndt, E. Schonbrunn, D.A. Harki, W.C. Pomerantz

MEDI 39. Identification of a novel DYRK1A inhibitor lead from computational modeling of kinase inactive conformations. **K. Kumar**, P.M. Ung, P. Wang, H. Wang, H. Li, M.K. Andrews, A. Stewart, A. Schlessinger, R. deVita

MEDI 40. Trifluoromethyl oxetanes: Synthesis and evaluation as a *tert*-butyl isostere in the gamma secretase modulator program. **P. Mukherjee**, C. am Ende, M. Pettersson, J.K. Dutra, L. Xie

MEDI 41. Highly selective dopamine D_3 receptor (D_3R) antagonists with arylated diazaspiro alkane cores. **S. Reilly**, S. Griffin, M. Taylor, K. Sahlholm, C. Weng, K. Xu, R.R. Luedtke, R.H. Mach

MEDI 42. Discovery of new indomethacin-based analogs with potentially selective cyclooxygenase-2 inhibition and observed diminishing to PGE2 activities. **S.E. Kassab**, M.A. Khedr, H. Ali, M.M. Abdalla

MEDI 43. Withdrawn.

MEDI 44. Utilizing small molecule adjuvants to increase colistin efficacy against Gram-negative bacteria. **B. Minrovic**, C. Melander

MEDI 45. Assessment of mitochondrial membrane potential in cells and *in vivo* using click chemistry and mass spectrometry. **K. Shaffer**, R.A. Smith, M.P. Murphy

MEDI 46. Discovery of reactive oxygen species inducer for treatment of lung cancer. **F. Ndombera**

MEDI 47. Development of novel penicillin binding protein 2 (PBP2) inhibitors as drug candidates for penicillin- and cephalosporin-resistant *Neisseria gonorrhoeae*. **J.M. Turner**, P.M. Woster, C. Davies

MEDI 48. 1,2,4-triazolidine-3-thiones as narrow spectrum antibiotics against *Acinetobacter baumannii*. **W. Huggins**, C. Melander

MEDI 49. Nitrogen-containing derivatives of *O*-trimethyl-2,3-dehydrosilybin: Design, synthesis, and *in vitro* evaluation in prostate cancer cell models. **B. Vue**, S. Zhang, A. Vignau, G. Chen, X. Zhang, Q. Chen

MEDI 50. Discovery of hydroxylated benzofuro[3,2- b]pyridin-7-ol derivatives as DNA topoisomerase inhibitors: Synthesis, biological evaluation and structure-activity relationship study. **A. Shrestha**, **T.M. Kadayat**, G. Bist, T.B. Thapa Magar, P. Katila, Y. Kwon, E. Lee

MEDI 51. Evaluation of serotonin modulators as a novel treatment for inflammatory bowel disease. **D.J. Canney**, **B.E. Blass**, K. Blattner, R. Gao, J. Gordon, H. Wang, W. Khan, D. Pippin

MEDI 52. Applying EPSA in guiding permeability optimization of small molecules. **K. Song**, R. Romero

MEDI 53. Towards understanding the unbound state of drug compounds: Implications for the intramolecular reorganization energy upon binding. **I. Chen**

MEDI 54. Examination of proteins bound to nascent DNA in mammalian cells using: BrdU-ChIP-Slot-Western technique. **D. Pablito**, S. Bhaskara

MEDI 55. Structure–activity relationship of a tetrahydroisoquinoline class of N–methyl–D–aspartate receptor modulators that potentiates GluN2B–containing N–methyl–D–aspartate receptors. **M.**

‡*Cooperative Cosponsorship*

Epplin, K.L. Strong, J. Bacsa, C.J. Butch, P.B. Burger, D.S. Menaldino, S. Traynelis, D. Liotta

MEDI 56. Synthesis and biological effects of a novel carborane-based β-amino acid for the treatment of glioblastoma. **T. He**, S.V. Chittur, R. Musah

MEDI 57. Synthesis of novel CCR1 antagonists for treatment of glioblastoma. **F. Faizal**, K. Mack, E. Shepherd, S. Chakravorti, M. Gill, M. Notarmaso, I. Pabon, N. Patel, H. Rao, J. Yarfi, J. Xie, J.R. Merritt

MEDI 58. (1-4)-*S*-thiodisaccharides: Potential anticancer drug candidates against human malignant gliomas. J. Sarnik, M. Toma, A. Czubatka-Bienkowska, A. Macieja, T. Sliwinski, **Z.J. Witczak**, R. Bielski, T. Poplawski

MEDI 59. HPLC detection of ferulic acid, gallic acid and quercetin from aqueous extracts of *Moringa oleifera*. **A.G. Gonzalez**, A. Mar, H.M. Morales

MEDI 60. Synthesis of JMS-17-2 and its analogs as new potential CX3CR1 antagonists. **M. Gao**, M. Wang, J.A. Meyer, J.S. Peters, H. Zarrinmayeh, P. Territo, G.D. Hutchins, Q. Zheng

MEDI 61. Developing structure-phototoxicity relationships for the better prediction of phototoxicity. **T. Takai**, Y. Dragan, R. Naven

MEDI 62. Resurrecting aged acetylcholinesterase to combat organophosphorus poisoning. **N. Rigel**, S. Davis, A.J. Franjesevic, B. Scarpitti, Q. Zhuang, C.S. Callam, C.M. Hadad

MEDI 63. Design and synthesis of dual ALK/BRD4 inhibitors. **E. Watts**, E. Tucker, D. Heidenreich, B. Bellenie, S. Knapp, L. Chesler, S. Hoelder

MEDI 64. Discovery of IACS-6274: A potent, selective GLS1 inhibitor with excellent pharmacokinetic properties under development for cancers with specific metabolic vulnerabilities. **M.J. Soth**, K. Le, G. Liu, J.P. Burke, J.J. Kovacs, J.P. Bardenhagen, C.A. Bristow, B. Czako, C. Carroll, M.E. Di Francesco, M.M. Hamilton, M. Geck-Do, A. Harris, V. Giuliani, Y. Jiang, T. Johnson, Z. Kang, Z. Liu, T. McAfoos, M. Miller, W.S. Palmer, N.E. Rogers, H.E. Shephard, N.D. Spencer, J. Theroff, A. Yau, G. Draetta, T. Heffernan, C. Toniatti, P. Jones

MEDI 65. Discovery of novel bicyclic pyridone derivatives as inhibitors of EZH2. **M.A. Marx**, **T.P. Bobinski**, D.M. Briere, J.G. Christensen, R.A. Galemmo, M.R. Lee, N. Sudhakar, J.W. Winkelman

MEDI 66. Potent small-molecule inhibitors of tubulin polymerization targeted for selective release mediated by tumor-associated hypoxia. **Z. Shi**, R. Guddneppanavar, B.A. Winn, C. George, T.E. Strecker, Y. Wang, J. Gerberich, A. Winters, E. Lin, C.J. Maguire, J. Ford, D.J. Chaplin, R.P. Mason, M.L. Trawick, K.G. Pinney

MEDI 67. Development and screening of new cathepsin B and K inhibitors utilizing substituted thiosemicarbazones. **R. McConnell**, H. Sarepalla, P. Akula, B. Guda, D. Yermala, N. Kadasala, K. Sayyar, W. Godwin, L. Wen

MEDI 68. Development and screening of new cathepsin D inhibitors. **R. McConnell**, K. Malayala, K. Yarlagadda, K. Sayyar, C. Trana, W. Godwin, L. Wen

MEDI 69. Lead optimization of cathepsin K inhibitors for disease-modifying osteoarthritis. **A. Ginnetti**, D. Paone, K. Nanda, A. Green, C.S. Burgey, L. Duong, H. Glantschnig, L. Huang, P. Lu, S. McElwee-Witmer, R. Vogel, N. Wei, G. Wesolowski, S. Carroll, S. Mosser, R. Robinson, S. Adamski, D. Eular, N. Hatcher, B. Luo, L. Lubbers, H. Webber, k. wessner, K. Anderson, S. Crathern, D. Dooney, J.D. Ellis, Y. Kuo, B. Ma, D. Rudd, B. Wan, C. Wudarski, M. Zrada, S. Stachel

MEDI 70. Small molecules inhibitors of PCSK9-LDLR protein-protein interaction. J. Taechalertpaisarn, **C.M. Serrano**, B. Zho, X. Liang, K. Burgess

MEDI 71. Using in-line ion-exchange impurity scavenging to improve flash purification efficiency. **J.R. Bickler**

MEDI 72. Lead optimization of novel CETP inhibitors for cardiovascular diseases. **G. Park**, S. Kim, H. Hwang, E. Lee, S. Woo, E. Ko, C. Im, S. Lee, W. Lee, M. Ma, S. Lee, M. Song

MEDI 73. Histone H3 and H4 acetylation of gamma-globin gene induced by phenylsulfonylfuroxan. **J.L. Dos Santos**, T.R. Melo, C. Kumkhaek, C. Lanaro, K.P. Barbieri, M.E. Lopes-Pires, R.C. Chelucci, I.Z. Carlos, S. Marcondes, K. Chegaev, S. Guglielmo, L. Lazzarato, R. Fruttero, M. Chung, G.P. Rodgers, F.F. Costa

MEDI 74. Design and synthesis of novel peroxisome proliferator-activated receptor β agonists. **K. Jung**, K. Kim, S. Cho, J. Chin

MEDI 75. Cyclohexyl GPR40 full agonists for the treatment of Type 2 diabetes. **S.K. Meegalla**, J. Lanter, H. Huang, S. Lee, T. Martin, J. Silva, M. Otieno, B. Rady, L. Norquay, J. Xu, J. Qi, M. Rankin, Y. Wang, S. Zhao, E. Arnoult, Y. Gong, J. Liu, X. Fran, F. Du, S. Lohani, A. Pocai, M.R. Player

MEDI 76. Imidazopyridazine analogues as anti-malarial PfPI3K inhibitors. **R. Liu**, T. Pandharkar, I. Safeukui, S. Bhattacharjee, H. Liu, O. Wiest, K. Haldar, M.J. Miller

MEDI 77. Structure based drug design in the search of selective inhibitors of the plasmepsin V (PmVPf) from *Plasmodium falciparum*. **W. Ferraz**, G.M. Ferreira, G.H. Trossini

MEDI 78. Design and synthesis of new peptide-benznidazole conjugates targeting *Trypanosoma cruzi* fibronectin receptor. P. Pitasse-Santos, D. Decoté-Ricardo, C.G. Freire-de-Lima, A.K. Giri, V.J. Hruby, **M.E. Freire De Lima**

MEDI 79. Identification of ligand-efficient inhibitors of *Trichomonas vaginalis* uridine nucleoside ribohydrolase using NMR-based fragment screening. **S. Auletta**, W. Caravan, J. Persaud, D.G. Brown, D.W. Parkin, B.J. Stockman

MEDI 80. Ribavirin selectively inhibits the guanosine/adenosine/cytidine nucleoside hydrolase from *Trichomonas vaginalis*. **W. Caravan**, R. Alam, A. Barbarovich, M. Ismail, A. Barskaya, D.W. Parkin, B.J. Stockman

MEDI 81. Emerging SAR for several series of *Trichomonas vaginalis* adenosine/guanosine preferring nucleoside ribohydrolase inhibitors derived from fragment analog screening. **J.A. Gonzalez**, A. Kaur, V. Sapojnikov, D.G. Brown, D.W. Parkin, B.J. Stockman

MEDI 82. Organizing 3D project data for structure-based drug design. **E. Metwally**

MEDI 83. MOEsaic: Application of matched molecular pairs to interactive SAR exploration. **A. Ajamian**

MEDI 84. Multi-target molecular profiling using MOE: A CYP450 isoform selectivity case study. **M.R. Goldsmith**

MEDI 85. Exploiting solvent effects in drug design and optimization. **C. Williams**

MEDI 86. Problem based learning with MOE. **A. Bonin**

MEDI 87. Total synthesis and analogue development of the cyclic imine natural product scytonemide A. **R.J. Tokarski**, T. Wilson, J.E. Orjala, H.L. Rakotondraibe, J. Fuchs

MEDI 88. Using small-molecule structural chemistry to inform drug discovery: Applications of the Cambridge Structural Database. **P. Sanschagrin**, S. Sekharan

MEDI 89. Behavior and biological significance of caseinolytic protease P in *Clostridium difficile*. **N. Lavey**, A.S. Duerfeldt

MEDI 90. Development and construction of an original compound library for CNS drug discovery: Combining computational and wet data to enhance CNS drug-likeness. **D. Hasegawa**, P.P. Graczyk, R. Nicewonger, G.S. Bhatia, L. Birch, P. Dimopoulos, A.H. Payne, Y. Kobayashi, T. Terauchi, R. Clark, S. Suzuki, M. Watanabe, T. Nishioka, H. Terauchi, S. Ozaki, I. Kushida, T. Suh, M.J. Yu, F. Benayoud, K. Sanders, F. Fang

MEDI 91. Bicyclic pro-drug S1P1 partial agonists: Exploring olefinic side chains to modulate the PK, PD, and toxicology profiles. **M. Yang**, Z. Xiao, T. Dhar, H. Xiao, J.L. Gilmore, A. Mathur, J. Xie, K. McIntyre, T. Taylor, X. Yang, L. Lehman-McKeeman, H. Sun, A.M. Marino, G. Cornelius, D. Shen, M. Cvijic, L. Salter-Cid, P.H. Carter, A.J. Dyckman

MEDI 92. Evolution of AMPK activators with improved muscle exposure. **J. Hicks**, D. Feng, J. Apgar, R. Wilkening, L. Wei, K.J. Leavitt, J. Dropinski, L. Chu, X. Qian, A. Kekec, G. Dong, A. Kim, H. Lu, H. Guan, K. Lu, X. Yang, J. Gorski, G. Eiermann, A. Gollapudi, M. Kurtz, M. Trujillo, R. Myers, D. Kemp, M. Hu, S. Xu, I.K. Sebhat

MEDI 93. Short acting pan-AMPK activators as exercise mimetics. **J. Apgar**, R. Wilkening, L. Wei, K.J. Leavitt, D. Feng, H. Lu, H. Guan, K. Lu, X. Yang, J. Gorski, G. Eiermann, A. Gollapudi, M. Kurtz, M. Trujillo, R. Myers, D. Kemp, M. Hu, S. Xu, I.K. Sebhat

MEDI 94. Design and synthesis of NR analogues to inhibit glucose metabolism in cancer cells. **E. de las Heras Ruiz**, S. Butterworth, I. Stratford, R. Bryce, A.P. Thomas, D. Stead

MEDI 95. How relevant is secondary structure mimicry in design of small molecules to disrupt protein-protein interfaces? J. Taechalertpaisarn, **M. Arancillo**, C. Lin, R. Lyu, Z. Jiang, L.M. Pérez, T.R. Ioerger, K. Burgess

MEDI 96. Finding conserved residue triplets on protein-protein interfaces. **R. Lyu**, K. Burgess

MEDI 97. Small molecule peptidomimetic to perturb protein-protein interactions targeting NEDD8-NAE. **C. Lin**, K. Burgess

MEDI 98. Cleavable, targeted small-molecule maytansinoid conjugate improves therapeutic index on treating metastatic breast cancer. **Z. Jiang**, K. Burgess

MEDI 99. Near-infrared zwitterionic dye to target TrkC expressing cancer cells. **S.M. Usama**, K. Burgess

MEDI 100. Withdrawn.

MEDI 101. Mechanism of inhibition of *Mycobacterium tuberculosis* isocitrate lyase by 3-nitropropionate. **S. Ray**, D. Kreitler, A.M. Gulick, A.S. Murkin

MEDI 102. Potentiation of *para*-aminosalicylic acid (PAS) by chemical inhibition of *para*-aminobenzoic acid (PABA) biosynthesis in *Mycobacterium tuberculosis*. **S. Dawadi**, Y. Minato, A.D. Baughn, C.C. Aldrich

MEDI 103. Repurposing of antipsychotic drugs as anti-tuberculosis agents. **J. Schultz**

MEDI 104. Cephalosporin-pyrazinoic acid conjugates: Novel agents for drug-resistant tuberculosis. **M. Cole**, J. Buonomo, Y. Minato, J. Thiede, A.D. Baughn, C.C. Aldrich

MEDI 105. Teixobactin: A recently discovered antimicrobial peptide. Structure–activity relationship. **B.G. de la Torre**, S.A. Abdel Monaim, Y.E. Jad, E.j. Ramchuran, A. El-Faham, F. Albericio

MEDI 106. Natural product inspired drug discovery from *Clerodendrum colebrookianum* Walp.: Fragment-based drug design, synthesis and testing for anticancer activity. **H. Arya**, C.S. Yadav, S.B. Syed, S. Kannadasan, M. Coumar

MEDI 107. Synthesis and pharmacological evaluation of histone deacetylase inhibitors as fetal hemoglobin inducers. **J.L. Dos Santos**, A.C. Melchior, P.L. Bosquesi, A.R. Pavan, C. Lanaro, M. Chung, R. Rusinova, R.C. Chelucci, O.S. Andersen, F.F. Costa

MEDI 108. Improved UV detection of peaks during elution with absorbing solvents. **J.E. Silver**, D. Johnson, C. Bailey, S. Paeschke, R. Lewis

MEDI 109. Identification of bicyclic hexafluoroisopropyl alcohol sulfonamides as RORβt/RORc inverse agonists. Employing structure-based drug design to improve PXR selectivity. **H. Gong**, D.S. Weinstein, Z. Lu, J. Duan, S.M. Stachura, L. Haque, A. Karmarkar, H. Hemagiri, D. Raut, A. Gupta, J. Khan, D. Camac, J. Sack, A.T. Pudzianowski, D. Wu, M. Yarde, D. Shen, V. Borowski, J. Xie, H. Sun, C. D'Arienzo, M. Dabros, M.A. Galella, F. Wang, C.A. Weigelt, Q. Zhao, W. Forster, J.E. Somerville, L.M. Salter-Cid, J.C. Barrish, P.H. Carter, M. Dhar

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MEDI 110. Understanding the structure and reactivity of the C-S linkage in biologically active 5-arylthio-5Hchromenopyridines. K.A. Grice, R. Patil, A. Ghosh, J. Paner, M. Guerrero, E. Camacho, P. Sun Cao, A. Niyazi, S. Zainab, R. Sommer, G. Waris, **S. Patil**

MEDI 111. Liquid biopsy: The simplest technique for pancreatitis and pancreatic cancer detection. **O. Covarrubias-Zambrano**, M. Kalubowilage, A.P. Malalasekera, H. Wang, S.O. Wendel, D.L. Troyer, S.H. Bossmann

MEDI 112. Machine learning consensus scoring improves performance across targets in structure-based virtual screening. S.S. Ericksen, H. Wu, H. Zhang, L. Michael, M. Newton, F.M. Hoffmann, **S.A. Wildman**

MEDI 113. Design and synthesis of novel deuterated $GABA_A$R-β6 subtype selective ligands with improved metabolic stability and enhanced bioavailability. **D.E. Knutson**, R. Kodali, M.R. Stephen, R.S. Verma, C. Witzigmann, M.A. Meirelles, N.M. Zahn, A.T. Huber, L. Arnold, M.M. Savic, M. Ernst, W. Sieghart, J.M. Cook

MEDI 114. Development of highly potent and selective inhibitors of DNA repair by 8-oxoguanine DNA glycosylase (OGG1). **Y. Tahara**, E.T. Kool

MEDI 115. Short and efficient access to very large non-peptidic macrocyclic space and applications to difficult targets. **A. Doemling**

MEDI 116. Virtual screening and MCR-based synthesis and characterisation of multiple scaffolds against p53-MDM2. **A. Doemling**

MEDI 117. Cystic fibrosis transmembrane conductance regulator protein (CFTR) correctors: Discovery and synthesis on THP series. **B. Liu**, X. Searle, C. Yeung, A. Bogdan, A. Swensen, A. Singh, C. Balut, Y. Fan, A. Manelli, T. Vortherms, C. Tse, P.R. Kym, X. Wang

MEDI 118. Addressing the transient subpocket of tRNA-guanine transglycosylase (TGT) with an acetylenic vector. **L. Movsisyan**, C. Hohn, W. Goetzke, E. Hassaan, G. Klebe, F.N. Diederich

MEDI 119. Human CAR activators as sensitizers of cyclophosphamide-based treatment for lymphomas. D. Liang, L. Li, **H. wang**, **F. Xue**

MEDI 120. Withdrawn.

MEDI 121. Quantitative structure-activity relationship applied of a series of 2-anilinobenzamide derivatives as Sirtuin-2 selective compounds hematological cancers candidates. **G.H. Trossini**, G.M. Ferreira, J.G. Magalhães, V.G. Maltarollo, F. Emery

MEDI 122. Discovery of novel KDM4B inhibitors to target periodontal disease progression. **J. Kirkpatrick**, J.M. Turner, R. Wilkinson, B. Harbin, K.L. Kirkwood, P.M. Woster

MEDI 123. Opportunities for advanced computational modeling to greatly accelerate drug discovery. **R. Abel**, S. Bhat, S. Mondal

MEDI 124. New inhibitors of BRD4 identified by combining fragment-based and HTS approaches. P. Borysko, O. Vasylchenko, S. Zozulya, **Y. Moroz**

MEDI 125. Antimelanoma studies of novel pyrazole and fused thiazoline-androstanedione derivatives. **C. Williams**, J. Whitt, C. Okolo, M.A. Alam

MEDI 126. Design and synthesis of novel OSW-1 scaffolds as precision cancer therapeutic agents. **A.T. Le**, **C. Malinky**, A. Burgett

MEDI 127. Design, synthesis, and evaluation of selective inhibitors of mono-(ADP-ribosyl)transferase, PARP-10. **C. McCadden**, R. Grant, A. Thorsell, J. Holechek, R. Lease, T. Karlberg, H. Schuler, D. Ferraris

MEDI 128. Design, synthesis and evaluation of PARP14 inhibitors as biological probes for target validation. **K. Upton**, A. Thorsell, T. Karlberg, M. Meyers, J. Holechek, R. Lease, H. Schuler, D. Ferraris

MEDI 129. Rational design and synthesis of potent and aqueous soluble bis-amino alcohol dimeric naphthoquinones with activity against acute myeloid leukemia cells. **E. Williams**, **R. Palmer**, B. Carter-Cooper, S. Dash, P. Truong, A. Emadi, R. Lapidus, D. Ferraris

MEDI 130. Synthesis and evaluation of novel belactosin A/carfilzomib hybrids as proteasome inhibitors. N.K. Dunlap, **M. Yadab**, C. Moss, K. Sampuda, L. Boyd

MEDI 131. Structural modifications of the N-terminal Hx-moiety in HxIP: Effects on DNA binding, cellular uptake, and gene expression. V. Satam, L. Pett, P. Patil, J. Sweers, M. Bowerman, S. Tzou, K. Olson, M. Lee, K. Kiakos, J. Hartley, **M. Lee**

MEDI 132. Synthesis of PSB-12054 and its analogs as new potential P2X4 receptor antagonists. M. Wang, **M. Gao**, J.A. Meyer, J.S. Peters, H. Zarrinmayeh, P. Territo, G.D. Hutchins, Q. Zheng

MEDI 133. Discovery of novel 5-oxa-2,6-diazaspiro[3.4]oct-6-ene derivatives as potent, selective, and orally available somatostatin receptor subtype 5 (SSTR5) antagonists for treatment of type 2 diabetes mellitus. **H. Hirose**, T. Yamasaki, T. Yamashita, M. Ogino, R. Mizojiri, N. Takakura, S. Morimoto, T. Nakahata, A. Kina, Y.O. Tamura, J. Sugama, H. Yashiro, Y. Muraki, Y. Nakano, A. Hata, T. Odani, Y. Shimizu, S. Iwasaki, M. Watanabe, T. Maekawa, S. Kasai

MEDI 134. Discovery of furanone derivatives as potent BRAF inhibitors. **D. Liu**, J. Zhang, R. Shen, L. Yang, J. Wang, L. Zhang, A. Gong, B. Lu, Y. Yan, Q. Sun, H. Wan, P. Yan, L. Zhang, J. Cao, M. Zhang

MEDI 135. Amino acids derived multifunctional N-, S-doped carbon dots for biomedical applications. **S. Sagbas**, **C. Silan**, **N. Sahiner**

MEDI 136. Adenosine-functionalized biodegradable PLA-B-PEG nanoparticles block osteoarthritis in rats. **X. Liu**

MEDI 137. Marine natural product manzamines as novel *Herpes simplex* virus type-1 inhibitors. J.R. Palem, **M. Mudit**, S.V. Hsia, K.A. El Sayed

MEDI 138. Design, synthesis and application of novel building blocks to "Escape the Flatland" in medicinal chemistry. **P. Mykhailiuk**, Y. Dmytriv, I. Komarov

MEDI 139. [2+2]-Photochemical synthesis and application of bicyclic amines: Advanced building blocks for medicinal chemistry. T. Dryzhenko, A. Denisenko, **P. Mykhailiuk**

MEDI 140. Synthesis and application of unnatural Proline analogues: Advanced building blocks for medicinal chemistry. V. Dolovanyuk, I. Kondratov, **P. Mykhailiuk**

MEDI 141. *In vitro* drug release studies for the treatment of TNBC and pancreatic cancers from natural derivated polymeric micro- and nano-particles. F. Comert Onder, S. Sagbas, M. Ay, B. Ozpolat, **N. Sahiner**

MEDI 142. Design, synthesis, and bioactivity of small molecule leads for the treatment of oculovascular diseases. **X. Dou**, D. Nath, G. Deng, Y. Shin, J. Ma, A.S. Duerfeldt

MEDI 143. Aryl galactosides targeting FmlH antagonists for the treatment of urinary tract infections (UTIs). **A. Maddirala**, V. Kalas, R. Chugani, M.E. Hibbing, J.S. Pinkner, S.J. Hultgren, J.W. Janetka

MEDI 144. Coumarin-based analogues of schweinfurthins. **C.M. Schroeder**, P. Dey, J.A. Beutler, D.F. Wiemer

MEDI 145. Synthesis and biological evaluation of 2,7-difluoropyronins. **B.E. Walls**, F. Boumelhem, Z. Woydziak

MEDI 146. Discovery of the orally-active irreversible LSD1 inhibitor 1-morpholino-3-(4-(((1R,2S)-2-phenylcyclopropyl) amino)piperidin-1-yl)propan-1-one (MRTX1519) with antitumor activity. **M.A. Marx**, R.M. Aranda, D.M. Briere, J.G. Christensen, L.D. Engstrom, P. Olson, N. Sudhakar, A. Vaisburg, J.W. Winkelman

MEDI 147. DYRK1A inhibition simultaneously targets amyloid-beta and tau pathology. **C. Foley**, C. Branca, D. Shaw, R. Belfiore, V. Gokhale, A. Shaw, B. Meechoovet, B. Smith, T. Dunckley, A. Caccamo, S. Oddo, C. Hulme

MEDI 148. Pharmaceutical applications of polyethoxyethylglycinamide (PEE-G) dendrimers. **R. Shrestha**, P. Rendle

MEDI 149. Hybrid BisQACs: Biscationic quaternary ammonium compounds merging the structures of two commercial antiseptics. **S.A. Schallenhammer**, R. Kontos, B. Bentley, S. Duggan, K. Morrison, W. Wuest, K.P. Minbiole

MEDI 150. Toward the discovery of PET radiotracer for imaging TDP-43 aggregates in FTD and ALS patients. **C. Boudou**, V. Darmency, T. Seredenina, J. Kocher, J. Stoehr, H. Kroth, A. Purohit, D. Paterson, L. Martarello, A. Pfeifer, A. Muhs

MEDI 151. Synthesis, structure activity relationship studies and biological evaluation of novel and selective 1*H*-pyrrolo[2,3-*b*] pyridine-2-carboxamides as related phosphodiesterase 4B (PDE4B) inhibitors. **A. K Vadukoot**, S. Sharma, C. Hopkins

MEDI 152. Bivalent probes to elucidate the mechanism of opioid enhanced neuroAIDS. **B. Falls**, H. Wang, D. Selley, K. Hauser, Y. Zhang

MEDI 153. "Magic methyl effect" in medicinal chemistry and methylation of (hetero)arenes. L. Hu, X. Liu, **Y.A. Liu**, X. Liao

MEDI 154. Prep LC: How much can I load? **J.E. Silver**, C. Bailey, D. Johnson, S. Paeschke, R. Lewis

MEDI 155. Computational analysis and synthesis of potential inhibitors active against Gram-negative bacteria. **R. Roldan**, A.O. Pajarillo, C.P. Embry, M.L. Cafiero, L.W. Peterson

MEDI 156. Withdrawn.

MEDI 157. Development of glutathione *S*-transferase (GST) covalent inhibitor. **Y. Shishido**, F. Tomoike, Y. Kimura, K. Kuwata, T. Yano, K. Fukui, H. Fujikawa, Y. Sekido, Y. Murakami-Tonami, T. Kameda, S. Shuto, H. Abe

MEDI 158. Synthesis and characterization of poly(Naringin) particles as new biomaterials. **M. Sahiner**, D.A. Blake, N. Sahiner

MEDI 159. Triazol-3-yl benzamides as potent and selective inhibitors of human factor XIIa. **R.A. Al-Horani**, D.K. Afosah

MEDI 160. Optimization of niclosamide analogs against enzalutamide resistant prostate cancer: Application in medicinal chemistry. **B. Kang**, Q. Zhong, M. Mottamal, M. Bratton, C. zhang, G. Wang, F. Payton-Stewart

MEDI 161. Design, synthesis and molecular modeling of new *N*-4-piperazinyl ciprofloxacin thiadiazole derivatives with antimycobaterial activity. H.H. Mohammed, **S.H. Abbas**, E.M. Abdelhafez, G.A. Moustafa, K.N. Dalby, **T.S. Kaoud**, G. Hauk, J.M. Berger, S. Mitarai, M. Arai, G.A. Abuo-Rahma

MEDI 162. Synthesis of fused and isolated triazoles based on thieno[2,3-*d*] pyrimidines and the screening of their PDE 5 inhibitory activity. M.A. Ameen, E.K. Ahmed, **M. Ramadan**, K.N. Dalby, **T.S. Kaoud**

MEDI 163. Anti-inflammatory properties of synthetic chalcones and Δ^1-pyrroline-5-carbonitriles. C. Aikens, E. Mazzio, V. Mihaylova, D. Tasheva, B. Mochona, K. Redda, **N.N. Mateeva**

MEDI 164. Inhibition of breast cancer cell growth and proliferation by novel synthetic Δ^1-pyrroline-5-carbonitriles and flavonoids. C. Aikens, V. Mihaylova, D. Tasheva, E. Mazzio, B. Mochona, K. Redda, **N.N. Mateeva**

MEDI 165. Synthesis and structure-activity relationship of β-quaternary phenylalanine analogs as LAT1 substrates. **B. Venteicher**, **C. Hall**, J. Campbell, C. Hernandez, A. Flint, H. Chien, K. Giacomini, C. Colas, A. Schlessinger, A.A. Thomas

MEDI 166. Optimization of LAT1 affinity for meta-substituted phenylalanine analogs. **S. Springer**, L. Stoner, K. Finke, A. Anthony, A. Flint, J. Bauer, C. Hernandez, H. Chien, K. Giacomini, C. Colas, A. Schlessinger, A.A. Thomas

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MEDI 167. Novel quinoline-incorporating 1,2,4-triazole/oxime hybrids inhibit STAT3 phosphorylation and suppress human melanoma cell growth. **D. Abdelhamid**, A.M. Mohassab, H.A. Hassan, M. Abdel-Aziz, K.N. Dalby, **T.S. Kaoud**

MEDI 168. Designing tet enzyme inhibitors to enhance learning and memory. **J. Alp**, **G. Chua**, **K. Wassarman**, H. Sun, C.P. Gettens, K. Zengeler, A. Kennedy

MEDI 169. Synthesis of conformationally restricted scaffolds by Double-Mannich reaction of cyclic ketones. **P. Mykhailiuk**, **Y. Moroz**

MEDI 170. Synthesis of novel unique pyrrolidines by [3+2]-cycloaddition of azomethine ylides with electron-deficient alkenes. **P. Mykhailiuk**, **Y. Moroz**, **O. Gavrylenko**

MEDI 171. Rapid access to novel multifunctional spirocyclic cores for drug discovery. **P. Mykhailiuk**, **Y. Moroz**, O. Gavrylenko

MEDI 172. Approaches to synthetically feasible polyfunctional building blocks. **P. Mykhailiuk**, O. Michurin, **Y. Moroz**

MEDI 173. ToxPHACTS – Toxicological read across using the Open PHACTS Discovery Platform. J. Gurinova, B. Knasmueller, L. Richter, D. Digles, **G.F. Ecker**

MEDI 174. K4DD-db – An open access resource for data on ligand binding kinetics. B. Knasmueller, L. Richter, **G.F. Ecker**

MEDI 175. Discovery of highly selective LRRK2 inhibitors as tool compounds to assess CNS PET tracer feasibility. **L. Tong**, Z. Zeng, G.J. Thomas, W. Li, D. Hesk, B. Wood, M. Ellis

MEDI 176. Synthesis of aminoacid ester prodrugs of BW-AQ-238 as potential inhibitors of MDM2/MDM4 dimerization to induce apoptosis in cancer cells. **A. Anifowose**, Z. Yuan, X. Yang, A. Draganov, B. Wang, L. Gu, S. Yi, T. Liu, M. Zhou

MEDI 177. Biophysical investigation of transcription factor Erg-DNA binding properties and the inhibition of Erg by small molecules. **B. Liu**, G.M. Poon, A.A. Farahat, A. Kumar, D.W. Boykin, W. Wilson

MEDI 178. Discovery of highly potent, selective, covalent inhibitors of JAK3. **J. Kempson**, D. Ovalle, J. Guo, S. Wrobleski, S. Lin, S. Spergel, J. Duan, B. Jiang, Z. Lu, J. Das, B.V. Yang, J. Hynes, H. Wu, J.S. Tokarski, J. Sack, J. Khan, G.L. Schieven, L. Salter-Cid, A. Fura, Y. Blatt, J.C. Barrish, P.H. Carter, W.J. Pitts

MEDI 179. Fused thiazoline-androstane derivatives as potential anticancer agents. C. Okolo, J. Whitt, C. Williams, **M.A. Alam**

MEDI 180. High affinity dopamine D4 receptor subtype-selective ligands as molecular tools to study addiction. **C.A. Boateng**, M. Day, R. Free, K. Stewart, D. Sibley, T. Keck

MEDI 181. Sulfonamide motif in NMDA receptor ligands. **S. Summer**, D.S. Menaldino, S. Traynelis, D. Liotta

MEDI 182. Alpha7 nicotinic acetylcholine receptor silent agonists: Exploration of the SAR for NS6740. **M. Pismataro**, C. Stokes, R. Papke, N. Horenstein, C.M. Dallanoce

MEDI 183. Negative allosteric modulators of the cannabinoid receptor 2: Protein modeling, binding site identification and molecular dynamics simulations in the presence of an orthosteric agonist. **P. Pandey**, K. Roy, R.J. Doerksen

MEDI 184. Computational analysis of adduct formation between benzaldehyde derivatives and DNA. **E. Voytsekhovskaya**, D.J. Marell, D.R. Quirk Dorr

MEDI 185. Intuitive workflow to enumerate and explore large virtual libraries. **M.D. Segall**, A. Cooke, J. Chisholm, E. Champness, P. Hunt, T. Mansley

MEDI 186. Dual inhibition of Bcl-2/Mcl-1 and MDM2 with novel β-helix mimetics based on a densely-functionalized isoxazole core. **I.L. Conlon**, A. Falat, N. Bowen, S. Fletcher

MEDI 187. Covalent strategies towards the selective inhibition of the Mcl-1 oncoprotein. **N. Bowen**, G. Njoku, M. Sun, W. Yu, A.D. Mackerell, S. Fletcher

MEDI 188. Structure-based design of dual Bcl-2/Mcl-1 inhibitors. **G.E. Vickers**, B. Drennen, S. Fletcher

MEDI 189. Rational design of spiro-thiazine-based selective BACE1 inhibitors: Targeting the flap to gain selectivity over BACE2. **K. Kusakabe**, K. Fujimoto, N. Asada, E. Matsuoka, K. Fuchino, H. Ito, D. Moechars, H. Gijsen

MEDI 190. Development of novel casein kinase 1d inhibitors for treatment of Alzheimer's disease. **V. Jha**, S. Kauloorkar, M. Bratton, C. Gettridge, H.M. Duong, R. Schroeder, J. Sridhar

MEDI 191. Identification and *in vivo* evaluation of Liver X receptor b-selective agonists for the potential treatment of Alzheimer's disease. **S. Stachel**, K.K. Nanda, M.T. Rudd, E. Brnardic, S. Suon, M. Cosden, K. Wessner, C. Zerbinatti, J. DiMuzio, J. Maxwell, J. Uslaner, M. Michener, P. Szczerba, W. Wuelfing, Y. Yuan, J. Ballard, M. Holahan, M.T. Bilodeau, J. Renger, D. Klein, V. Uebele, J. Lu, G. Parthasarathy, Z. Wu

MEDI 192. Novel *in silico* strategies towards optimization of new anthrax antitoxin leads. **C.M. McDermott**, E.A. Ambrose

MEDI 193. Incorporation of tetracycline in water ethanol bentonite dispersions. **M. Bobadilla**, E. Moura, M.S. Valenzuela, F. Valenzuela

MEDI 194. Choline geranate deep eutectic solvents exhibiting unique antimicrobial activity against *Staphylococcus aureus*. **S. Ottavi**, K.A. Bidle, D.L. Jacobs

MEDI 195. Synthesis of anti-cancer drugs to inhibit P-gp pumping action. **M.A. Aljowni**

MEDI 196. Synthesis and optimization of a near-infrared fluorescent choline kinase β inhibitor: Cyclo-JAS239. **R. Humeidi**, A. Arroyo, S. Osharovich, A.V. Popov, E. Delikatny

MEDI 197. Label-free visualization of peptides and small molecules in tumor explants using mass spectrometry imaging. **B. David**, O. Dubrovskyi, J.M. Frasor, L.M. Sanchez, T.W. Moore

MEDI 198. Synthesis and antimicrobial evaluation of 3-hydroxy-2-oxindole natural products and derivatives. G.M. Dominguez, M.L. Morshead, J.D. Shapiro, C.P. Lyndaker, **M.M. Majireck**

MEDI 199. Withdrawn

MEDI 200. 3-Aminopyrazoles as type I and type II inhibitors for p38β MAP kinase. **N.J. Vantangoli**, D.W. Boerth, S. Rasapalli

MEDI 201. Optimization of NK-kB inducing kinase inhibitors: A fragment based approach. **N. Scorah**, W. Keung, L. Kwok, P. Tanis, M. Sabat, D. Lawson, J. Ermolieff, N. Ishii

MEDI 202. Janus kinase 1/3 (JAK1/3) inhibitors: Improving selectivity against Rho kinase 1 (ROCK1) in a series of piperidinylaminopyrrolo[1,2-b]pyridazine-3-carboxamides. **M.E. Mertzman**, S. Spergel, G. Brown, B.V. Yang, S. Lin, J.S. Tokarski, J.S. Lippy, R.F. Zhang, M.A. Galella, S. Pitt, J. Sack, J. Khan, P.H. Carter, J.C. Barrish, S.G. Nadler, L.M. Salter-Cid, G.L. Schieven, S. Wrobleski, W.J. Pitts

MEDI 203. Withdrawn

MEDI 204. Identification and optimization of second generation CDK2 inhibitors as otoprotectants against cisplatin-induced ototoxicity. **R. Hazlitt**, T. Teitz, J. Min, J. Bonga, D. Currier, T. Chen, Z. Rankovic, J. Zuo

MEDI 205. Inhibition of *Neisseria meningitidis* by 5'-sulfonamide-nucleoside conjugates. **M. Ghali**, **V. Lopez**, **M. Hight**, A. Awad

MEDI 206. Investigating the use of mixed stationary phases for peptide purification via reversed phase flash chromatography. **E. Denton**, **J.R. Bickler**

MEDI 207. Synthesis and analysis of a folate conjugate for simultaneous capture and detection of cancer cells. **W.A. Henne**

MEDI 208. Development of a *Coxiella burnetii* culturing method for high throughput assay to identify growth inhibitory small molecules. **M. Khan**, M. Hale

MEDI 209. Design and synthesis of hydroxylated 2-phenyl-4,6-dithienyl/furanylpyridines as selective topoisomerase IIβ inhibitors. **P. Katila**, G. Bist, T.B. Thapa Magar, A. Shrestha, Y. Kwon, E. Lee

MEDI 210. Synthesis and characterization of de-sulfonylated product of Rigosertib, a late phase III clinical candidate. **M.R. Mallireddigari**, V. Dandu, V. Bharathi, B. Akula, V. Pallela, S.C. Cosenza, C. Ren, M. Maniar, P. Reddy, M. Reddy

MEDI 211. Molecular dynamics simulations of the epsilon unit in HBV pgRNA. **R.P. Pemberton**

MEDI 212. Near-IR cyanine optical/PDT theranostic for TrkC+ breast cancer. **J.P. Shrestha**, K. Burgess

MEDI 213. SAR study of novel FABP inhibitors as antinociceptive, anti-inflammatory, and anticancer agents. **S. Yan**, M. Elmes, M. Awwa, J. Li, K. Ziadkhanpour, M. Kaczocha, D. Deutsch, I. Ojima

MEDI 214. Chemo-enzymatic synthesis of "clickable" and photoactive NAADP analogs for identification of the NAADP receptor. **P. Su**, J. Bretz, T. Asfaha, C. Trabbic, T. Walseth, J. Slama

MEDI 215. Structure activity relationship studies of indole-containing heterocycles targeting lipid regulation pathways. **H. Xie**, K. Yang, G.N. Winston-Mcpherson, W. Tang

MEDI 216. Targeting lipid regulation pathways by novel small molecules. **K. Yang**, H. Xie, G.N. Winston-Mcpherson, D. Stapleton, M. Keller, A. Attie, W. Tang

MEDI 217. Binding of silymarin flavolignan isomers to human serum albumin: Experimental and computational studies. D. Hlangothi, **K. Anthony**, M.A. Saleh

MEDI 218. Chemoenzymatic synthesis of novel O-linked glycopeptide cancer vaccine candidates. **J. Zhang**

MEDI 219. Synthesis and evaluation of 7-O-aminoalkyl-3,3',4'-O-trimeylfisetins as anti-prostate cancer cell agents. **M. Lee**, K. Muthima, X. Li, G. Chen, Q. Chen

MEDI 220. Nitrogen-containing derivatives of tertramethylquercetins: A new group of anti-prostate cancer agents. **P.S. Rajaram**, Z. Jiang, A. Phasakda, A. Rivera, G. Chen, Q. Chen

MEDI 221. Synthesis of N-(9-acridinyl)-O-phenylhydroxylamines as anti-cancer agents. **C.I. Muldoon**, A.L. Johnson, M.D. Mosher

MEDI 222. Identification of conserved waters in macromolecular structures using ProBiS H2O. **M. Jukic**, J. Konc, S. Gobec, D. Janezic

MEDI 223. Suppressive effect of benzoxazinoids on prostate cancer cells. **B. Bhattarai**, P.L. Gregersen, M.T. Skaanild, I.S. Fomsgaard

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Rooms 252-254

Impact of Small-Molecule Breakthrough Therapies on Human Health

N.A. Meanwell, P.M. Scola, K. Yeung, *Organizers, Presiding*

8:30 Introductory Remarks.

8:35 MEDI 224. Breakthrough therapies–FDA perspective. **D. Matecka**

9:10 MEDI 225. Discovery and development of alectinib, a selective and potent ALK inhibitor for treatment of ALK-positive advanced non-small cell lung

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cancer. **K. Kinoshita**

9:45 MEDI 226. Discovery of oliceridine (TRV130), a novel G protein biased ligand at the μ-opioid receptor, for the management of moderate to severe acute pain. **A.L. Crombie**, X. Chen, F. Skobieranda, D.G. Soergal, J. Violin, M. Lark

10:20 MEDI 227. US FDA breakthrough designation: Impact and benefits on the development of TAGRISSO™ (osimertinib). **B. Barlaam**, R. Finlay, R. Ward

10:55 MEDI 228. Targeting the cause of cystic fibrosis: Recent progress. **P. Grootenhuis**

Section B
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

Recent Advances in the Discovery of Deubiquitinase Inhibitors

E.F. DiMauro, E.R. Strieter, *Organizers, Presiding*

8:30 MEDI 229. Selenocysteine as a latent bioorthogonal probe for deubiquitylating enzymes. **C. Chatterjee**

9:00 MEDI 230. Chemical approach to manipulate the protein degradation machinery for human health. **B. Lee**, R. King, D. Finley

9:30 MEDI 231. Targeting the deubiquitinase STAMBP inhibits NALP7 inflammasome activity. **J. Bednash**, N. Weathington, J. Londino, M. Rojas, D. Gulick, B.B. Chen, R.K. Mallampalli

10:00 Intermission.

10:15 MEDI 232. Targeting DUBs in hematological malignancies. **S. Buhrlage**, E. Weisberg, I. Lamberto, X. Liu, N. Schauer, J. Yang, S. Dhe-Paganon, H. Seo, J. Griffin, V. DeCesare, S. Ritorto, M. Trost

10:45 MEDI 233. Target selection and small molecule development in the DUB space. **M. Clague**

11:15 MEDI 234. Fragment guided path to a selective inhibitor of USP7 and its implications for chain linkage specificity. **T. Maurer**

11:45 MEDI 235. Reactive site-centric chemoproteomics identifies a new class of deubiquitinase enzymes. **I.E. Wertz**

12:15 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Rooms 255-257

Emerging Therapeutics: Gasotransmitters

L.M. Berreau, P.K. Mascharak, *Organizers*
B. Wang, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 MEDI 236. Releasing and sensing reactive sulfur species. **M. Xian**

8:35 MEDI 237. New strategies for carbonyl sulfide (COS) and hydrogen sulfide (H_2S) delivery. **M.D. Pluth**

9:05 MEDI 238. Discovery and clinical evaluation of MK-8150, a novel nitric oxide donor with a unique mechanism of nitric oxide release. **A. Ali**

9:35 MEDI 239. Development of novel hydrogen sulfide donors to treat cardiovascular diseases. **D. Lefer**, Z. Li, J. Kang, M. Xian

10:05 Intermission.

10:20 MEDI 240. Carbon monoxide is hepatoprotective through generation of nitric oxide. **L. Otterbein**, D. Gallo, S. Otterbein, X. Ji, B. Wang, B. Zuckerbraun, S. Robson

10:50 MEDI 241. Inhibition of cystathione beta-synthase by CO in human breast cancer cells: Implications in chemotherapeutic drug sensitivity. **P.K. Mascharak**

11:20 MEDI 242. Flavonol-based carbon monoxide releasing molecules. **L.M. Berreau**

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Rooms 252-254

Identifying Selective PI3K Inhibitors

G. Phillips, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 MEDI 243. Identification of alpelisib as a selective inhibitor of PI3Kβ. **R.A. Fairhurst**, G. Caravatti, V. Guagnano, P. Imbach-Weese, R. Mah, M. Gerspacher, I. Bruce, P. Furet, M. Knapp, C. Fritsch, C. Schnell, F. Blasco, J. Blanz, H. Seiler

2:10 MEDI 244. Discovery of two clinical candidates as isoform selective PI3K inhibitors: AZD8835 a potent and selective inhibitor of PI3Kβ/β and AZD8186 a potent and selective inhibitor of PI3Kβ/β for the treatment of cancers. **B. Barlaam**, S. Cosulich, S. Degorce, B. Delouvrie, M. Fitzek, H. Germain, S. Green, U. Hancox, C. Harris, K. Hudson, C. Lambert-van der Brempt, M. Lamorlette, A. Le Griffon, J. Lohmann, M. Maudet, R. Morgentin, G. Ouvry, K. Page, G. Pasquet, M. Pasquet, A. Peru, P. Ple, L. Ruston, T. Saleh, M. Vautier, M. Walker, L. Ward, N. Warin

2:40 MEDI 245. Discovery of isoform-selective inhibitors of PI3K in a series of propeller-shaped compounds. **L. Patel**

3:10 MEDI 246. Exploration and enhancement of PI3Kdelta selective compounds: The discovery of Nemiralisib and beyond. **K. Down**

3:40 MEDI 247. Discovery of potent and selective inhibitors of PI3Kgamma and production of a roadmap for selectivity design. **P. Collier**

4:10 MEDI 248. Discovery of taselisib. **T.P. Heffron**

Section B
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

Advancing Clinical Candidates from Phenotypic Screening

A.K. Cheung, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 MEDI 249. Chemotype–phenotype–target. **H. Waldmann**

2:05 MEDI 250. Discovery of CFTR modulators for the treatment of cystic fibrosis. **S.S. Hadida-Ruah**

2:35 MEDI 251. *In vivo* translatability: Lessons learned from a phenotypic screen designed to identify small molecules that selectively decrease endogenous c-MYC protein levels in cancer cells. **J.R. Medina**

3:05 Intermission.

3:20 MEDI 252. Phenotypic drug discovery: Probing emerging biology to delivering clinical candidates. **A. Plowright**, J. Lillie, P. Mason, E. Makino

3:50 MEDI 253. From here to there: Recognizing paths leading to treatments for spinal muscular atrophy and other diseases. **M.G. Woll**, G.M. Karp, N.A. Naryshkin, A. Dakka, A.A. Branstrom, J. Narasimhan, L. Cao, Y.C. Moon

4:20 MEDI 254. Proteasome inhibitors: A single cure for multiple kinetoplastid diseases. **A.S. Nagle**, V. Molteni, F. Supek

4:50 Panel Discussion.

Section C
Ernest N. Morial Convention Center
Rooms 255-257

2018 MEDI Young Investigators Symposium

T.E. Prisinzano, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 MEDI 255. Small molecule disruptors of the GK-GKRP interaction. **K. Ashton**

2:05 MEDI 256. Immune modulation by butyrophilin ligands and their prodrugs. **A.J. Wiemer**

2:35 MEDI 257. Discovery and SAR evolution of a novel class of selective adenosine A_{2A} antagonists for the treatment of Parkinson's disease. **Y. Lim**, G. Gallo, M.M. Lo, E. Metzger, B.R. Whitehead, Q. Deng, H. Wang, Y. Yu, R. Anand, R. Hodgson, L. Hyde, D. Mullins, D. Prelusky, E. Parker, A.W. Stamford, A. Ali

3:05 MEDI 258. Discovery of small molecule and nucleic acid inhibitors of APOBEC3 deaminases. **D.A. Harki**

3:35 MEDI 259. Generating selective inhibitors of methionine-gatekeeper kinases: Case studies on NIK, PAKs and PKD1. **S.T. Staben**, J. Feng

4:05 MEDI 260. Optimization of non-covalent Nrf2 activators for use in models of chronic wound healing. **T.W. Moore**, B. David, B.G. Richardson, A.D. Jain, L. Chen, L.A. DiPietro, S. Reddy, H. Potteti

4:35 Concluding Remarks.

Advances in Molecular Recognition of Double-Helical DNA & RNA
Sponsored by CARB, Cosponsored by MEDI and ORGN

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Large-Scale Applied Molecular Modeling
Sponsored by COMP, Cosponsored by CINF and MEDI

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
A.W. Stamford, *Organizer*

8:00–10:00

33, 38, 39, 47-48, 63, 101, 104, 114-115, 122, 126-127, 146, 152, 159, 165, 167, 189, 192, 204, 221. See previous listings.

322-325, 330, 332, 338, 347, 349, 353, 358, 384, 389, 400, 409, 411. See subsequent listings.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

Remarkable Women of Medicinal Chemistry
Cosponsored by PROF and WCC
P.L. Ornstein, A.S. Ripka, *Organizers, Presiding*

8:30 Introductory Remarks.

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8:35 MEDI 261. There and back again: Therapies for the treatment of obesity and diabetes. **A.E. Weber**

9:10 MEDI 262. From organic chemistry to the discovery of PET ligands. **C.D. Jesudason**

9:45 MEDI 263. Malaria drug discovery: How medicinal chemistry and global responsibility intersect. **S.S. Canan**

10:20 MEDI 264. Novel and atypical DAT inhibitors for the treatment of psychostimulant use disorders. **A.H. Newman**

10:55 MEDI 265. From bench to clinic: The discovery of GDC-0853 a potent, selective and reversible Btk inhibitor. **W.B. Young**

11:30 MEDI 266. Science of medicinal chemistry in the discovery of medicines: From ideas-to-trenches-to-the corner office-to-medicine cabinet. **N.T. Zaveri**

Section B
Ernest N. Morial Convention Center
Rooms 252-254

Eyeing Effective Treatment for Retinal Diseases with Small Molecules

T.P. Heffron, *Organizer, Presiding*

8:30 MEDI 267. Strategies to deliver small molecules to the retina by topical drops: A paradigm shift. **A.K. Mitra**, A. Mandal, K. Cholkar

9:10 MEDI 268. Optimizing ophthalmic drug delivery strategies to enhance efficacy: Modeling, formulation technology, and ◦BCS. **H. Gukasyan**

9:40 MEDI 269. PI3K inhbitors for the treatment of retinal diseases. **T.P. Heffron**

10:10 Intermission.

10:25 MEDI 270. Design, synthesis, and evaluation of nonretinoid retinol binding protein 4 antagonists for the potential treatment of atrophic age-related macular degeneration and Stargardt disease. **C.L. Cioffi**, N. Dobri, E. Freeman, M.P. Conlon, P. Chen, D. Stafford, D. Schwarz, K. Golden, L. Zhu, D.B. Kitchen, K. Barnes, B. Racz, Q. Qin, E.L. Michelotti, C.L. Cywin, W.H. Martin, P. Pearson, G. Johnson, K. Petrukhin

10:55 MEDI 271. Structure-based design of small-molecule Factor D inhibitors targeting the alternative complement pathway. **A. Vulpetti**, S. Randl, S. Ruedisser, N. Ostermann, P. Erbel, A. Mac Sweeney, B. Gerhartz, F. Cumin, C. Dalvit, K. Anderson, U.A. Argikar, S. Liao, E. Lorthiois, J.K. Maibaum

11:25 MEDI 272. Drug discovery on a challenging target: inhibiting the alternative complement pathway with small molecule factor B inhibitors. **H. Sellner**

Section C
Ernest N. Morial Convention Center
Rooms 255-257

General Orals

A.W. Stamford, *Organizer*
G. Wang, *Presiding*

8:30 MEDI 273. Synthesis and optimization of novel inhibitors targeting *M. tuberculosis* polyketide synthase 13 thioesterase domain. **R.C. Dhakal**, A. Aggarwal, M.K. Parai, R. Shrestha, A. Acharya, J.C. Sacchettini

8:55 MEDI 274. Orally-active inhibitors of H-PGDS for the treatment of asthma, allergic rhinitis and chronic obstructive pulmonary disease. **S. Thurairatnam**

9:20 MEDI 275. Optimization of the chemical matter and synthesis leading to a ketohexokinase inhibitor clinical candidate. **A.C. Smith**, S.B. Coffey, M.S. Dowling, D.P. Fernando, K. Futatsugi, K. Huard, T.V. Magee, B. Raymer, A. Shavnya, A.S. Tsai, M. Tu, H.M. Wisniewska

9:45 MEDI 276. Withdrawn.

10:10 MEDI 277. RMC-4550: An allosteric inhibitor optimized for *in vivo* studies of SHP2. **A.L. Gill**, N. Aay, A. Buckle, M.A. Goldsmith, A. Jogalekar, G. Kiss, E.S. Koltun, A. Marquez, K. Mellem, K. Mordec, R.J. Nichols, M. Saldajeno-Concar, C. Semko, M. Singh, J.A. Smith, N. Tibrewal, C. Tzitzilonis, Z. Wang, D. Wildes, S.E. Wilson, W. Won

10:35 MEDI 278. ASTX660, the first fragment-derived IAP antagonist in the clinic. **C. Griffiths-Jones**

11:00 MEDI 279. Rapid development of potent and selective CBP inhibitors: The impact of a tetrahydroquinoline LPF binder. **S.M. Bronner**

11:25 MEDI 280. Discovery and characterization of ingrezza (valbenazine): A VMAT2 inhibitor approved for the treatment of tardive dyskinesia. **N.D. Harriott**, J.P. Williams, E. Smith, H. Bozigian, D.E. Grigoriadis

11:50 MEDI 281. Strategies and challenges on the GluN2A-selective NMDA PAM program: A perspective on positive allosteric modulator (PAM) drug discovery. **M. Volgraf**

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Advances in Molecular Recognition of Double-Helical DNA & RNA
Sponsored by CARB, Cosponsored by MEDI and ORGN

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Jürgen Bajorath
Sponsored by COMP, Cosponsored by CINF and MEDI

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

MEDI Awards Symposium

A.W. Stamford, *Organizer*
P.L. Ornstein, *Presiding*

1:30 MEDI 282. Award Address (George and Christine Sosnovsky Award for Cancer Research Sponsored by the George and Christine Sosnovsky Endowment Fund). Anticancer drug discovery, for pets and people. **P.J. Hergenrother**

2:15 MEDI 283. Award Address (ACS Award for Team Innovation Sponsored by the ACS Corporation Associates). Discovery and development of Ibrance®, a first-in-class CDK4/6 inhibitor. **P.L. Toogood**, D.W. Fry, N. Do, V.G. Beylin, B.P. Chekal, N.D. Ide, B.P. Jones, H. Zhou

3:00 MEDI 284. Leveraging diverted total synthesis to elucidate the mechanism of action of a pseudomonad-specific antibiotic. **W.M. Wuest**

3:30 MEDI 285. HIV-1 drug discovery: Inhibitors of virus attachment and virion maturation. **N.A. Meanwell**

4:00 MEDI 286. Drug discovery in academia. **M.E. Jung**

4:30 Introduction of Awardee.

4:35 MEDI 287. Award Address (Alfred Burger Award in Medicinal Chemistry Sponsored by Gilead Science Inc.). Discovery and development of novel therapeutics for treating viral diseases, cancers, and inflammatory disorders. **D. Liotta**

Section B
Ernest N. Morial Convention Center
Rooms 252-254

Boron in Medicinal Chemistry & Chemical Biology

R. Moreira, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 MEDI 288. Towards boron based antibiotics and beta-lactamase inhibitors. **C. Schofield**

2:05 MEDI 289. Translating new chemical space to new function: The case of BN/CC isosterism in biomedical research. **S.Y. Liu**

2:35 MEDI 290. Boron heterocycles: Studies on their properties and applications in drug discovery and chemical biology. **D.G. Hall**, B. Akgun, M. Boghi

3:05 Intermission.

3:20 MEDI 291. Boroscan: An enabling technology for the discovery of bioactive molecules containing boron. **A.K. Yudin**

3:50 MEDI 292. Exploring iminoboronates in the assembly of reversible bioconjugates. **P.M. Gois**

4:20 Concluding Remarks.

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in honor of Seth B. Herzon

Sponsored by ORGN, Cosponsored by MEDI

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Discovery of Small Molecules Targeting RNA
Sponsored by ORGN, Cosponsored by CARB and MEDI

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Jürgen Bajorath
Sponsored by COMP, Cosponsored by CINF and MEDI

TUESDAY EVENING

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

First Time Disclosure of Clinical Candidates

J.B. Schwarz, *Organizer, Presiding*

9:00 MEDI 293. Discovery of AZD0364, a potent and selective oral inhibitor of ERK1/2 that is efficacious in both monotherapy and combination therapy in models of NSCLC. **I. Simpson**, M. Anderton, D.M. Andrews, J. Breed, C. Cook, E. Davies, J.E. Debreczeni, H. Emtenas, V. Flemington, F.D. Gibbons, M.A. Graham, P.J. Hopcroft, T. Howard, J. Hudson, C. Jones, C.D. Jones, N. Lindsay, M. Malmgren, M. Osborne, J.E. Pease, S. Pithani, P. Rawlins, K. Roberts, S. St-Gallay, S. Swallow, M. Tonge, R. Ward

9:35 MEDI 294. GDC-0927, a selective estrogen receptor degrader and full antagonist for ER+ breast cancer. **X. Wang**

10:10 MEDI 295. Discovery of LSZ102, a potent, orally bioavailable selective estrogen receptor degrader (SERD) for the treatment of estrogen receptor positive breast cancer. **G. Tria**, T. Abrams, J. Baird, H.E. Burks, B. Firestone, L. Gaither, L.G. Hamann, G. He, C.A. Kirby, S. Kim, F. Lombardo, K.J. Macchi, D.P. McDonnell, Y. Mishina, J.D. Norris, J. Nunez, C. Springer, Y. Sun, N.M. Thomsen, C. Wang, J. Wang, B. Yu, C.T. Yip, S. Peukert

10:45 MEDI 296. Discovery of PRN1008: A reversible covalent BTK inhibitor for treatment of autoimmune diseases. **T.D. Owens**

‡*Cooperative Cosponsorship*

11:20 MEDI 297. Discovery of BMS-986195: A strategy for identifying a highly potent and selective covalent inhibitor providing rapid inactivation of Bruton's tyrosine kinase (BTK). **S.H. Watterson**, Q. Liu, D.G. Batt, M. Beaudoin Bertrand, W. Guo, H. Gong, S. Ahmad, L. Negash, K. Ngu, M. Pattoli, S. Skala, L. Cheng, M.T. Obermeier, R. Moore, R. Vickery, P.A. Elzinga, J. Dai, L. Discenza, C. D'Arienzo, K.M. Gillooly, T. Taylor, C. Pulicicchio, K.W. McIntyre, M.A. Galella, A. Tebben, J. Li, R. Zhao, D. Smith, R. Rampulla, A.J. Allentoff, M.A. Wallace, K.N. Voronin, A. Mathur, L. Salter-Cid, J.E. Macor, P.H. Carter, A. Fura, J.R. Burke, J.A. Tino

Section B
Ernest N. Morial Convention Center
Rooms 252-254

Discovery of Small Molecules Targeting RNA: Where Are We & Where Are We Going?
Cosponsored by CARB and ORGN
S.C. Zimmerman, *Organizer*
A.E. Hargrove, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 MEDI 298. Targeting G-quadruplexes in the Zika virus RNA genome. **C.J. Burrows**, A.M. Fleming, Y. Ding, N. Nguyen

8:30 MEDI 299. Structure and assembly of the U6 snRNP. E.J. Montemayor, A.L. Didychuk, Y. Nomura, G. Sidhu, A. Yake, D. Brow, **S. Butcher**

8:55 MEDI 300. Riboswitches as targets, models, and tools for small molecule-RNA interactions. **M. Hammond**

9:20 MEDI 301. High performance virtual screening by targeting a high-resolution RNA dynamic ensemble. **H.M. Al-Hashimi**

9:45 Intermission.

10:15 MEDI 302. Covalent mRNA labeling using fluorescent self-alkylating ribozymes. T. Ayele, S. Ellipilli, **J.M. Heemstra**

10:40 MEDI 303. Small-molecule covalent probes for study and control of RNA. **E.T. Kool**

11:05 MEDI 304. Structural studies of long non-coding RNAs and riboswitches. **K. Sanbonmatsu**

11:30 MEDI 305. Rational design of cell-permeable, multivalent ligands for repeat disease RNA. Y. Bai, J. Lee, U. Chembazhi, L. Hagler, S. Peng, E. Chan, A. Kalsotra, **S.C. Zimmerman**

11:55 Concluding Remarks.

Radiopharmaceutical Chemistry

Fluorine

Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

Structure-Based Drug Design for GPCRs
Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballrooms A/B

First Time Disclosure of Clinical Candidates

J.B. Schwarz, *Organizer, Presiding*

1:30 MEDI 306. Invention of INCB054329 and INCB057643, two potent and selective BET inhibitors in clinical trials for oncology. **A.P. Combs**

2:05 MEDI 307. Advances in understanding the relationship of pharmacology to GPCR structure and function: A GPR40 journey from the lab to diabetic patients. **C. Hamdouchi**

2:40 MEDI 308. Design, identification and clinical progression of RV521, an inhibitor of respiratory syncytial virus fusion. **G.S. Cockerill**, A. Bedernjak, D. Brookes, R. Dowey, R. Harland, S.M. Johnson, N. Mathews, M. Paradowski, M. Peeples, C. Scott, M. Steadman, G. Taylor, M. Thom, E. Thomas, S.E. Ward, D. Watterson, P. Young, K. Powell

3:15 MEDI 309. Discovery of VNRX-5133: A broad-spectrum serine- and metallo-beta-lactamase inhibitor (BLI) for carbapenem-resistant bacterial infections ("superbugs"). **C.J. Burns**, B. Liu, G. Chu, R. Trout, R. Jackson, D. McGarry, J. Hamrick, D. Daigle, S. Cusick, D. Pevear, L. Xerri

3:50 MEDI 310. Discovery and synthesis of JNJ-54861911, a novel orally active BACE1 inhibitor. **Y. Koriyama**, A. Hori, S. Yonezawa, T. Yamamoto, Y. Baba, H. Ito, A. Kato, G. Sakaguchi

Section B
Ernest N. Morial Convention Center
Rooms 252-254

General Orals

A.W. Stamford, *Organizer*
S. Cyr, *Presiding*

1:30 MEDI 311. Amphiphilic heterocyclic sulfonamides as carbonic anhydrase inhibitors with selectivity for tumor-overexpressed isozymes – towards theranostic systems for cancer detection and treatment. **M.A. Ilies**, S. Akocak, U. Mondal, C.T. Supuran

1:50 MEDI 312. Investigating the impact of covalency on PROTAC-mediated degradation of BTK. **H. Lithgow**, C. Tinworth, J.D. Harling, I. Smith, G. Burley

2:10 MEDI 313. Applications of protein-observed ^{19}F NMR (PrOF NMR) for inhibitor discovery of BET and non-BET bromodomains. **W.C. Pomerantz**

2:30 MEDI 314. Identification of potent, selective, cell-active class 1 histone deacetylase inhibitors lacking a zinc binding group. **D.C. Beshore**

2:50 MEDI 315. LAT1 membrane transporter: reevaluating the meaning of L and A. **A.A. Thomas**, H. Chien, A.A. Zur, K. Giacomini, C. Colas, a. schlessinger, L. Lin, K. Finke, E. Augustyn, S. Springer, L. Stoner, A. Flint, N. Heeren, L. Hansen, A. Anthony, C. Hernandez, B. Venteicher, J. Campbell, C. Hall

3:10 MEDI 316. Inhibition of nutrient acquisition and metabolism in pathogenic bacteria. **T.A. Wencewicz**

3:30 MEDI 317. Phospholipase A_2: A target for the development of anti-inflammatory agents. **V. Mouchlis**, E.A. Dennis, J. McCammon

3:50 MEDI 318. Fragment-based ligand design of carbohydrate receptor ligands. H. Baukmann, J. Schulze, R. Wawrzinek, J. Aretz, E. Wamhoff, M. Nazare, **C. Rademacher**

4:10 MEDI 319. Targeting myeloid differentiation using potent human dihydroorotate dehydrogenase (*h*DHODH) inhibitors designed by scaffold hopping using regio substituted hydroxyazole scaffolds. **M.L. Lolli**, S. Sainas, A.C. Pippione, D. Bonanni, M. Giorgis, E. Giraudo, E. Lupino, P. Goyal, M. Piccinini, R. Friemann, C. Garino, G. Saglio, A. Cignetti, V. Gaidano, P. Circosta, S. Al-Karadaghi, D. Boschi

4:30 MEDI 320. Discovery of benzimidazole derivatives as water-soluble CLK1/4 kinase inhibitors and their anticancer activity. **J. Cheong**, M. Zaffagni, B.R. Zetter, L. Sun

4:50 MEDI 321. Design, synthesis and application of clickable β-secretase photoaffinity probes for (off-)target identification. **C. am Ende**, A. Zuhl, C. Nolan, M.A. Brodney, S. Niessan, K. Atchison, C. Houle, D. Karanian, C. Ambroise, J. Brutlet, E. Beck, S. Doran, B.T. O'Neill, C. Change, K.F. Geoghegan, G. West, J. Judkins, X.J. Hou, D. Riddell, E.A. LaChapelle, D.S. Johnson

Radiopharmaceutical Chemistry

Carbon-11 & Radionuclide Production

Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

Structure-Based Drug Design for GPCRs
Sponsored by COMP, Cosponsored by CINF and MEDI

WEDNESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall B1

General Posters
Cosponsored by ORGN
A.W. Stamford, *Organizer*

7:00–9:00

MEDI 322. Design, synthesis and biological evaluation of hydrogen persulfide donors. **B. Yu**, Y. Zheng, B. Wang

MEDI 323. Long wavelength visible-light triggered hydrogen sulfide donors. **A. Sharma**, A. PK, H. Chakrapani

MEDI 324. Small molecule based tools for localized delivery of hydrogen sulfide. **P. Chauhan**, P. Bora, R. Govindan, S. Jos, H. Chakrapani

MEDI 325. Augmenting protein stability and function through hydrogen-bond-enhanced halogen bonds. **A.C. Carlsson**, M.R. Scholfield, R.K. Rowe, M.C. Ford, A.T. Alexander, R.A. Mehl, P.S. Ho

MEDI 326. Next generation antibiotics: Progress toward the synthesis of an enzyme-activated nitric oxide-releasing antimicrobial fluorescent prodrug. **H. Hibbard**, M.M. Reynolds

MEDI 327. Discovery and development of novel diazeniumdiolate derivatives as nitric oxide donors. **T.J. Henderson**, A. Ali, M.M. Lo, B.R. Whitehead, L. Yan, P. Huo, D. Cully, K. Mitra, Y. Li, S. Hoerrner, M.D. Weisel, L. Yang

MEDI 328. Comparison of NO donors, N-N-di-N'-butyl-1,6-hexanediamine and N-N-di-N'-propyl-1,6-hexanediamine, attenuating thrombogenicity in extracorporeal circuits. **M.M. Jeakle**, T. Johnson, T. Major, M.E. Meyerhoff, R. Bartlett

MEDI 329. Stimuli-activated metal-free CO prodrugs: A general strategy. X. Ji, Z. Pan, L. De La Cruz, **B. Wang**

MEDI 330. Cancer targeted nitric oxide delivery with a fluorescence reporter. **R. Govindan**, M. Bagheri, D.K. Saini, H. Chakrapani

MEDI 331. Organic CO prodrugs activated by endogenous ROS. **Z. Pan**

MEDI 332. Development of sulfur dioxide prodrugs with triggered release and tunable release rate. **W. Wang**, X. Ji, Z. Du, E. El-labbad, K. Ji, B. Wang

MEDI 333. Design, synthesis and biological evaluation of nitrate ester analogs of SCP-1. **M. Das**, N.G. Bazan, M.L. Trudell

MEDI 334. Immunostimulatory mannose derived glycoclusters as potential cancer therapeutics. R. Leino, E. Narvi, V. Kähäri, **J. Rahkila**, J. Markola, E. Veräjänkorva, K. Elenius, R. Ekambaram

MEDI 335. Design, synthesis and evaluation of novel sphingosine kinase 1 inhibitors with improved hydrophilic properties. S. Manore, J.C. Hurlbert, **T. Grattan**

MEDI 336. Fisetin sensitize the head and neck cancer (HNC) cells to radiation treatment *via* mitochondrial exchange inhibition. **R. Singh**, D. Tailor, D. Nambiar, **S.V. Malhotra**

MEDI 337. Synthesis of heterocyclic bioactive compounds. **M. Collins**, M.L. Henning, K. Elkin, N. Arai, K. Ohgo, D. Gilmore, J. Hershberger

MEDI 338. Discovery of a binding site hot spot for non-steroidal anti-inflammatory drugs on the cellular nucleosome. **A.M. Mfuh**

MEDI 339. Novel fluoroaryl acetamides: orally bioavailable lead compounds for the treatment of medically refractory epilepsy. **A. Dubrovskiy**, A.V. Krivoshein, J.L. Guevara, J. Renfrow, J. Jaimes

MEDI 340. Combined fluorescence and circular dichroism spectroscopic investigations examining the influence of buffer components on the stability and solubility of free and warfarin-bound serum albumins. G. Bishop, **Y. Satterwhite**, **S. Weber**, **R. Williams**, K.M. Bishop, L. Robinson

MEDI 341. Encapsulation of thioguanine anti-cancer drug by adsorption on microporous MOF Basolite A100 and its controlled release. C. Grinnell, **A. Samokhvalov**

MEDI 342. Molecular modelling,

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synthesis and bioactivity of peptide as anti-angiogenic and anti-dengue NS2B/NS3 protease inhibitors. **E.E. Kamarulzaman**, R. Vanderesse, A. Mohd Gazzali, M. Barberi-Heyob, C. Boura, C. Frochot, O. Shawkataly, M. Mohd Rawi, S. Mohamad, H.A. Wahab

MEDI 343. Novel levodopa-PAK-Tempo conjugate (LPTC) protects the heart against ischemia/reperfusion injury via inhibiting mitochondrial fission and oxidative stress. **S. Hou**

MEDI 344. Scaffold Hopping approach for the development of a potent class of allosteric HIV-1 integrase inhibitors. **T. Wilson**, N.T. Cockroft, J. Antwi, P. Koneru, M.J. Kobe, M. Kvaratskhelia, J. Fuchs

MEDI 345. Investigation of synthetic strategies for the development of heterocyclic small molecule HIV-1 integrase inhibitors. **N. Jentsch**, J. Sun, M.G. Donahue, J. Kessl

MEDI 346. Withdrawn.

MEDI 347. Synthesis and biological properties of pyridine-fused cyclotriazadisulfonamides (CADA) against HIV. **L. Lumangtad**, D. Schols, K. Vermeire, T.W. Bell

MEDI 348. Withdrawn.

MEDI 349. Synthesis and characterization of sulfonium silent agonists of the alpha 7 nicotinic receptor. **M. Quadri**, C. Stokes, A. Gulsevin, A. Felts, K.A. Abboud, R. Papke, N. Horenstein

MEDI 350. Advantages of an ocean of compounds over the usual fishing pond. **Y. Moroz**, C. Detering, O. Savych, C. Lemmen

MEDI 351. Towards selective inhibitors of the astacin proteases Meprin β and β. **D. Ramsbeck**, A. Hamann, K. Tan, D. Schlenzig, S. Schilling, M. Buchholz

MEDI 352. Composition and endogenous biosynthesis of the chemical defense of *Pyractomena borealis*. **D.A. Posner**

MEDI 353. Co-crystal technology for drug development. **S. Andree**, C.B. Aakeroy, A. Sinha

MEDI 354. Self-assembling peptide-nanosponges for cell-mediated cytotherapy. **A.S. Yapa**, M. Kalubowilage, H. Wang, P. Thapa, T.B. Shrestha, J. Yu, O. Covarrubias-Zambrano, M. Pyle, D.L. Troyer, S.H. Bossmann

MEDI 355. Bringing β-lactam antibiotics back to life: Strategies for restoring their activity against resistant bacteria. **M.A. Boudreau**

MEDI 356. Synthesis of berberine derivatives as potential antibiotics. **J. Rusnak**, L.M. Mori Quiroz, A. De Los Santos, M. Anyika, M.D. Clift

MEDI 357. Withdrawn.

MEDI 358. Targeting multiple myeloma: Toxicity elucidation and structural modification of 6-thiopurine and development of new targeting delivery systems. **R. Rafferty**, C.J. Weeramange, V. Hoang, A. Fatino

MEDI 359. Design, synthesis, and pharmacokinetic evaluation of 4-aminopyridones as glutaminase inhibitors of cancer cell metabolism. **J.P. Burke**, M.M. Hamilton, M. Han, Z. Kang, K. Le, Z.J. Herrera, H.E. Shephard, J.P. Bardenhagen, N.E. Rogers, Z. Liu, T. Johnson, Y. Jiang, J.J. Kovacs, M. Geck-Do, G. Draetta, T. Heffernan, C. Toniatti, P. Jones, M.E. Di Francesco, M.J. Soth

MEDI 360. Cucurbit[7]uril based main-chain polymer as drug carrier for supramolecular polymeric chemotherapy. **H. Chen**, Y. Chen, H. Wu, J. Xu, Z. Sun, X. Zhang

MEDI 361. New vacuolar-ATPase inhibitors as antiviral therapies. **A. Lindstrom**, D.P. Petrov, R. Davey, V.J. Davisson

MEDI 362. CRAFT'ing a human serum albumin-ligand screen: A CPMG relaxation-editing approach using ^{1}H NMR spectroscopy and complete reduction to frequency amplitude table (CRAFT) to characterize ligand binding to human serum albumin. **D.P. Soulsby**

MEDI 363. Discovery of bicyclic carboxamides as hepatitis B virus (HBV) core protein assembly modulators. **Y. Du**, N. Hwang, M.R. Campagna, S. Wu, J. Guo

MEDI 364. Synthesis and biological evaluation of novel long acting muscarinic antagonists. **J.F. Boulos**, **J. Baquier**

MEDI 365. Design and synthesis of thiophene-*N*-methylbenzimidazole diamidines exploiting the "β-hole" concept for specific recognition of DNA G-C base pairs. **A.A. Farahat**, A. Kumar, P. Guo, A. Paul, W. Wilson, D.W. Boykin

MEDI 366. Synthesis and biological evaluation of novel tumor-targeting biotin-linker-fluoro-taxoid conjugate. **Y. Jing**, C. Wang, X. Wang, I. Ojima

MEDI 367. Trisubstituted cyclohexanes as dual antagonists of CCR2 and CCR5. **R.J. Cherney**, D.G. Batt, G. Brown, S. Kumar, P. Anjanappa, Y. Zhang, S.S. Ko, A.S. Srivastava, J.V. Duncia, J.B. Santella, D. Gardner, R. Mo, A.V. Rose, J. Chen, J. Pang, S. Xu, M. Dabros, M.A. Galella, A. Mathur, M. Cvijic, J.C. Barrish, S. Mandlekar, Q. Zhao, P.H. Carter

MEDI 368. Regioselective synthesis of N-substituted pyrazoles. **N. Norman**, **T. Mello**, N. Kneitschel, D. Cheon, O. Moeller, A. Huang

MEDI 369. Facile synthesis of fucosylated peptides. **C. Gibbons**

MEDI 370. Nanomedicine for trans-epithelial oral delivery of ivermectin for Zika. **B. Surnar**, S. Dhar

MEDI 371. SAR of novel anti-fungal agents targeting the synthesis of fungal GlcCer. **K. Haranahalli**, Y. Sun, C. Lazzarini, J.E. Zambito, M. Del Poeta, I. Ojima

MEDI 372. Synthesis and biological activity of coumarin-containing prodrugs of a butyrophilin ligand. **N.M. Harmon**, B.J. Foust, C.C. Hsiao, A.J. Wiemer, D.F. Wiemer

MEDI 373. Reactive oxygen species (ROS) triggered 5-fluorouracil prodrugs. **Y. Ai**, O. Obianom, Y. Shu, F. Xue

MEDI 374. Identification and optimization of potent and selective RIPK2 inhibitors. **S. Nikhar**, G. Cuny, A. Degterev

MEDI 375. Design and synthesis of substituted 3-(*tert*-butylamino)-2-phenylpropanoate esters as potential dopamine transporter inhibitors. M. Cooper, **D. Dukes**, L.A. Bonner

MEDI 376. Synthesis of δ,δ-difluoromethyl halohydrins and their application in the synthesis of β-aminobutyric acid type B ($GABA_B$) receptor agonists. **M. Sowaileh**, R. Hazlitt, D.A. Colby

MEDI 377. Development of a practical synthesis of THC and CBD enabling access to novel analogs. **Z. Shultz**, J.W. Leahy, G. Lawrence

MEDI 378. Withdrawn.

MEDI 379. Synthetic study of orally available selective ASIC inhibitor. **K. Fujii**, H. Nakamura, Y. Umezaki, R. Takano, Y. Numata, T. Tanimoto, S. Wakimoto, L. Sitong, M. Izumi, T. Watanabe, T. Deguchi, T. Matsuo, T. Hirayama, S. Marumoto, M. Yoshida

MEDI 380. Emerging synthetic cannabinoids and their primary metabolites. **R.J. McKinnie**, C. Biggers, B. Euceda, T. Darweesh, X. Cao, M.L. Trudell

MEDI 381. Analysis of fluorescent thermal shift screening hits against *Burkholderia pseudomallei* IspF. **S.M. Watkins**, D.L. Grote, C.A. Muller, J.M. Blain, C. Luan, J.R. Horn, T.J. Hagen

MEDI 382. Discovery of tetrahydropyran derivatives as inhibitors of indoleamine 2,3-dioxygenase – *in silico* screen and structure-activity relationship studies. **J. Cheong**, F.E. Jernigan, L. Sun

MEDI 383. Transesterification and bacterial quorum sensing inhibition of β-keto esters. **S.M. Meschwitz** , R. Ruest

MEDI 384. Development of the phyllanthusmin class of natural products: SAR, mechanistic probes, and drug property optimization. **A.C. Huntsman**, A. Young, J.L. Woodard, H. Chai, Y. Ren, M.A. Phelps, A.D. Kinghorn, J.E. Burdette, J. Fuchs

MEDI 385. Lessons taken from the study of HCV-NS3 protease affinity to its NS4A cofactor at different conditions. **M.T. Khayat**, M.E. El-Araby, A.M. Omar, M. El-Faky, S.T. Arold, S. Soror, H. Asfour, A. Khayyat

MEDI 386. Design, synthesis and bio evaluation of novel liver X receptor ligands. **R. Komati**, M. Ndukwe, K. LaMark, K. Payne, M. Bratton, J. Sridhar, K.E. Riley

MEDI 387. Design, synthesis and bio evaluation of amido phthalimides as CDK9 and VEGF inhibitors. **R. Komati**, V.C. Miles, M.M. Ismail, H. McFerrin, J. Sridhar

MEDI 388. Amidophthalimides derivatives as CDK9 and VEGFR inhibitors. **L. Ha**, **F.J. Richard**, R. Komati, J. Sridhar

MEDI 389. PROTACs – Small molecule induced protein degradation. **M. Pettersson**, C.M. Crews

MEDI 390. Synthesis and biological studies of C1β-(aminoalkyl)carbapenem antibiotics. T.Q. Nguyen, **M. Alqurafi**, P.W. Thomas, Z. Sun, T. Durand-Reville, R. Iyer, A. Shapiro, A. Miller, N. Al-Kharji, J. Kim, M. Cox, O. Marx, B. Meshram, P. Nguyen, C. Jacobson, T. Kongara, C. Shi, T. Palzkill, W. Fast, R. Tommasi, J.D. Buynak

MEDI 391. Next generation small molecule inhibitors of 5'-Methylthioadenosinenucleosidase (MTN) as novel antimicrobial agents. J.H. Thurston, **L. Wayment**, M. Vitale-Sullivan, A. Tao, K. Cornell, D. Xu

MEDI 392. Synthesis and biological evaluation of new hybrids phthalimide-furoxan derivatives useful in the treatment of Alzheimer's disease. R.C. Chelucci, **D.E. Chiba**, M. Placeres, I.Z. Carlos, J.L. Santos, M. Chung

MEDI 393. Biochemical analysis of Guayacan and Huisache: Two potential medicinal plants for the treatment of diabetes. **M. Jimenez**, H.M. Morales, A. Mar, J. Lara

MEDI 394. Design and synthesis of new dibenzofuranol ether derivatives for human cytochrome P450 design and synthesis of new dibenzofuranol ether derivatives for human cytochrome P450. **M. Hill-Odom**, K. Bongay-Williams, T. Hill, E. Kantrow, N. Goyal, M. Foroozesh

MEDI 395. Identification of inhibitors of the *Pseudomonas aeruginosa* HasA/HasR protein-protein interaction. **G. Centola**, W. Jiang, K. Hom, A.D. Mackerell, A. Wilks, F. Xue

MEDI 396. Synthesis of analogues of nosokophic acid. **T.J. Tetrault**, D. Peña-Romero, M.A. Boudreau

MEDI 397. Examining the interactions of novel furoxans using techniques in chemical biology. **E. Tackie-Yarboi**

MEDI 398. Novel charge-reduced heparin derivatives revealed as direct allosteric inhibitors of thrombin. **E.C. de Souza**, I. Craciun, C.A. Kulkarni, R.J. Kerns

MEDI 399. Structure-based drug design, synthesis, and evaluation of peptidic inhibitors of thrombin-mediated activation of platelets aggregation. **C.C. Clement**

MEDI 400. Incorporation of therapeutic proteins into polyester nanofibers via protein-polyelectrolyte complexes. **A. Mancuso**, A. Sadek, N. Pillarella, K.S. Raja

MEDI 401. Polyester films/implants loaded with insulin-polyelectrolyte particles for the treatment of diabetes. **A. Mancuso**, N. Pillarella, K.S. Raja

MEDI 402. Identification of dual AAK1/GAK inhibitors as host-targeted antiviral agent. **N.R. Kapadia**, B. Zuercher, t. wiillson

MEDI 403. Chiral optical properties of kavalactones from root extracts of *kava-kava* assessed by combined experimental and computational methods. **G. Bishop**, L.C. Bishop, L.K. DeShetler, B. Herrington, K.M. Bishop, H. McAlexander

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MEDI 404. Chloromethyl verdazyls as novel spin probes for biological systems. **D.J. Brook**, A. Herrera

MEDI 405. Differential scanning calorimetry studies reveal the curious influence of buffer salts on the stability and aggregation of serum albumin. **S.I. Ngwudike**, G. Bishop

MEDI 406. Design, synthesis and cytotoxity of new quinoline/oxime hybrids. S.H. Abbas, M.E. Shoman, K.N. Dalby, **T.S. Kaoud**, **H.A. Hassan**

MEDI 407. Design and synthesis of potent and selective HDAC6 inhibitors. B. Vergani, G. Sandrone, D. Modena, F. Leoni, G. Caprini, G. Pavich, M. Lattanzio, M. Marchini, M. Pezzuto, M. Skorupska, P. Cordella, P. Pagani, P. Pozzi, R. Perego, C. Steinkuhler, G. Fossati, **A. Stevenazzi**

MEDI 408. Discovery of hydrazine-bearing selective HDAC inhibitor based on panobinostate: Structure-activity relationship, anti-tumor mechanism and pharmacokinetics study. **X. Li**, **C. Chou**

MEDI 409. Synthesis and biological evaluation of HDAC inhibitors with an imidazole-based metal-binding group. **S.M. Dlamini**, A. Al-Hamashi, A. Lateef, R. Koranne, M. Rashid, W. Taylor, V. Tillekeratne

MEDI 410. Withdrawn.

MEDI 411. Expanding the pharmacological toolkit to study the CXCR4 receptor by developing fluorescent probes. **S. Dekkers**, B. Caspar, S. Hill, S. Briddon, B. Kellam, M. Stocks

MEDI 412. Active-state cannabinoid 1 (CB1) receptor: Protein modeling and comparison to recently published X-ray structures of the inactive-state and active-state CB1 receptors. P. Pandey, A. Aderibigbe, K. Roy, **R.J. Doerksen**

MEDI 413. Identification of novel small-molecule bioactive compounds in Baltic amber. **E.A. Ambrose**, C.M. McDermott, J. Thomforde

THURSDAY MORNING

Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

THURSDAY AFTERNOON

Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

NUCL

Division of Nuclear Chemistry and Technology

A. Hixon, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Radiopharmaceutical Chemistry
(see *FLUO*, Tue, Wed, Thu)

SOCIAL EVENTS:

Social Hour, 6:00 PM: Tue

BUSINESS MEETINGS:

NUCL Business Meeting, 5:00 PM: Tue

NUCL Executive Committee Meeting, 5:00 PM: Sun

SUNDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Isotope Harvesting at Accelerator Facilities

T.A. Bredeweg, G.F. Peaslee, G. Severin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 NUCL 1. *In situ* isotope harvesting from the beam dump cooling loop at the Facility for Rare Isotope Beams (FRIB) with hollow fiber supported liquid membrane (HFSLM). **M.D. Scott**, L. Sutherlin, J. Schorp, J.D. Robertson

8:30 NUCL 2. Feasibility of harvesting radon and noble gas isotopes from the FRIB Beam Dump. **A. Visser**, N.D. Scielzo, S. Sangiorgio, G. Severin

8:55 NUCL 3. Evaluation of solid supports for isotope harvesting at Brookhaven Linac isotope producer (BLIP). **J. Fitzsimmons**, L. Muench, A. Younes, K. Kubbard, D.G. Medvedev, C.S. Cutler

9:20 NUCL 4. Astatine-211 from harvested radon at the upcoming Facility for Rare Isotope Beams. **G. Severin**, P. Abel, H. Clause, A. Visser

9:45 Intermission.

10:05 NUCL 5. Harvesting ^{48}V at a radioactive ion beam facility. **C.S. Loveless**, B. Marois, S. Ferran, J. Wilkinson, L.T. Sutherlin, G. Severin, J.A. Shusterman, N.D. Scielzo, M.A. Stoyer, D.J. Morrissey, J.D. Robertson, G.F. Peaslee, S.E. Lapi

10:30 NUCL 6. Production yields of ^{52}Fe from symmetric complete fusion-evaporation reactions. **S. McGuinness**, J. Wilkinson, M. Couder, S.E. Lapi, G.F. Peaslee

10:55 NUCL 7. Isotope harvesting of ^{88}Zr for neutron-capture cross-section measurements. **J. Shusterman**, N.D. Scielzo, P. Abel, H. Clause, S.E. Lapi, C.S. Loveless, S. McGuinness, E.B. Norman, G.F. Peaslee, J.D. Robertson, G. Severin, D.A. Shaughnessy, M.A. Stoyer, L.T. Sutherlin, K. Thomas, A. Tonchev

11:20 NUCL 8. Use of ^{149}Tb and ^{152}Tb in preclinical and clinical investigations: Its mass separation and subsequent application for imaging and therapy. **N. van der Meulen**, U. Koester, K. Johnston, C.E. Vermeulen, C. Umbricht, M. Benesova, R. Hasler, N. Gracheva, R. Schibli, A. Singh, R.P. Baum, C. Mueller

11:45 Concluding Remarks.

SUNDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Actinide Complexes & Nanoclusters
Cosponsored by INOR
K.E. Knope, *Organizer*
T. Forbes, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 NUCL 9. Quantum and classical approaches to probe the structural, dynamical and hydration properties of tetravalent actinide elements. **F. Real**, E. Acher, M. Masella, V. Vallet

1:35 NUCL 10. Quantum-mechanical studies of actinide complexes: Benchmarking of new methods, novel complexes and novel reactivity. **S.O. Odoh**, N.K. Dandu

2:05 NUCL 11. Properties of AnO_2^+ and the pK_a's of aqueous an cations in different oxidation states. **D.A. Dixon**, M. Vasiliu, D. Xia, A. Gomez, K.A. Peterson, J.K. Gibson

3:05 Intermission.

3:20 NUCL 12. Topology, stability, solubility, and dynamics of uranyl peroxide cage clusters. **P.C. Burns**

3:50 NUCL 13. Understanding isomerism in peroxide nanocapsules: Are other isomers possible? **P. Miro**

4:20 NUCL 14. Broad look at the energy landscape of nanoclusters and their transformations. **A. Navrotsky**

MONDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Actinide Complexes & Nanoclusters
Cosponsored by INOR
K.E. Knope, *Organizer*
T. Forbes, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 NUCL 15. Aging of actinide solid sources during multi-year exposure to environmental conditions. **B.A. Powell**

9:05 NUCL 16. Tetravalent actinides – from polymeric complexes to nanoparticles. **C. Hennig**

9:35 NUCL 17. Hydration of uranyl fluoride and a novel chemical pathway to uranyl peroxide. **M.C. Kirkegaard**, A. Miskowiec, M. Ambrogio, J. Langford, B. Anderson

10:05 Intermission.

10:20 NUCL 18. Actinide oxide and peroxide nanoclusters: Structure and environmental stability. L.R. Sadergaski, W. Stoxen, G. Sigmon, **A.E. Hixon**

10:50 NUCL 19. Probing the bonding in dimers of tetravalent cerium and actinide homologues. **V. Vallet**, S.L. Estes, M.R. Antonio, S. Skanthakumar, L. Soderholm

11:20 NUCL 20. Coordination polymer (CP) networks and molecular complexes of tetravalent actinides (Th, U, Np) with aromatic polycarboxylate ligands or polyoxometalate (POM) species. **T. Loiseau**, N.P. Martin, C. Volkringer, S. Duval, J. Maerz, A. Ikeda-Ohno

Section B
Embassy Suites New Orleans
Prytania Room

Young Investigators in Nuclear & Radiochemistry

R. Sudowe, *Organizer*
T.A. Bredeweg, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 NUCL 21. Commissioning the EMMA spectrometer at TRIUMF. **N.E. Esker**, B. Davids, M. Alcorta, K. Hudson, M. Williams

8:55 NUCL 22. Separation of Pb, Bi and Po by cation exchange resin. **K. Kmak**, D.A. Shaughnessy, J. Despotopulos

9:15 NUCL 23. Thermal analysis of lanthanide chelates for nuclear forensics. **S. Shahbazi**

9:35 NUCL 24. Recovering barium from strontium resin using chelating agents. **A. Sorcic**, D. McLain, R. Sudowe

9:55 NUCL 25. Exploring the effect of the diluent on trivalent *f*-element extraction by the di-alkyl acidic organophosphorus extractant HEH[EHP]. **T. Martin**, K.L. Nash

10:15 Intermission.

10:35 NUCL 26. Comparison the solvent extraction behavior of Re(VII) with Tc(VII). **L. Neill**, G. Parker, D.E. Wall, N. Wall

10:55 NUCL 27. Spectroscopic speciation studies and kinetic investigations on the actinide lanthanide SEParation process (ALSEP). **G. Picayo**, M.P. Jensen

11:15 NUCL 28. Sodium bismuthate solubility in nitric acid. **P. Prem**, S.P. Mezyk, B. Mincher

11:35 NUCL 29. Investigating formation and competitive exchange kinetics for DTPA complexed Eu ions in aqueous solution. **A. Miller**, K. Larsson, S.P. Mezyk

MONDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Actinide Complexes & Nanoclusters
Cosponsored by INOR
K.E. Knope, *Organizer*
T. Forbes, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 NUCL 30. Expanding the structural toolkit to characterize heavy actinide complexes. **R.J. Abergel**

1:45 NUCL 31. Synthesis and reactivity of multimetallic uranium nitrides. **M. Mazzanti**, M. Falcone, L. Chatelain

2:15 NUCL 32. Development of UF_6 research at ICCF: Purification, corrosion and novel compounds. **L. Jouffret**, J. Hiltbrunner, M. Dubois

2:45 NUCL 33. Hexavalent uranium, neptunium and plutonium nitrate complexes. **R. Wilson**, M.G. Autillo

3:15 Intermission.

3:30 NUCL 34. Supramolecular assembly and tuning of actinyl cations. **C.L. Cahill**, K. Carter, M. Kalaj

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4:00 NUCL 35. Exploring actinyl oxo reactivity: Macrocyclic neptunyl inclusion compounds. **M.C. Basile**, E. Cole, M. Pyrch, T. Forbes

4:30 NUCL 36. Complexation of dioxoactinide ions by aqueous-soluble Schiff bases – Effects on solvent extraction. **C.A. Hawkins**, C. Bustillos, R. Copping, I. May, M. Nilsson

Section B
Embassy Suites New Orleans
Prytania Room

Young Investigators in Nuclear & Radiochemistry

T.A. Bredeweg, *Organizer*
R. Sudowe, *Organizer, Presiding*

1:30 NUCL 37. Complexation of technetium(IV) with selected halides. **C. Eiroa Lledo**, L. Lecrivain, D.E. Wall, N. Wall

1:50 NUCL 38. Interrogating the role of water in metal ion extraction into room temperature ionic liquids. **M.L. Rigney**, M.L. Dietz, C.A. Hawkins

2:10 NUCL 39. Effect of matrix constituents on the separation of plutonium and americium from bone samples. **N. Nguyen**, R. Sudowe

2:30 NUCL 40. Sequential extraction techniques to investigate movement and bioavailability of soil contaminants. **I. McNabb**, R. Sudowe

2:50 NUCL 41. Radiolytic degradation of tributyl phosphate in the presence of uranium. **R. Ngelale**, M. Nilsson

3:10 Intermission.

3:30 NUCL 42. Separation of actinium from thorium using polyoxometalates. **J. Hatcher**, A. Younes, J. Fitzsimmons, B.P. Burton-Pye, H. Cicek, C.S. Cutler, L.C. Francesconi

3:50 NUCL 43. Development of a radiotherapeutic nanoparticle for infection. **L.T. Sutherlin**, J.D. Robertson

4:10 NUCL 44. ^{72}As a candidate for PET imaging: From production to *in vivo* imaging. **V.A. Sanders**, A.J. DeGraffenreid, M. Gao, N. Turkman, J. Kim, C.S. Cutler

4:30 NUCL 45. Synthesis and *in vitro* evaluation of ^{99m}Tc/^{186}Re-cyclized somatostatin receptor-targeting peptides for the diagnosis/therapy of neuroendocrine tumors. **G. Makris**, J. Wang, M. Kuchuk, F. Gallazzi, S.S. Jurisson, H.M. Hennkens

4:50 Concluding Remarks.

TUESDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Actinide Complexes & Nanoclusters
Cosponsored by INOR
K.E. Knope, *Organizer*
T. Forbes, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 NUCL 46. Metal-ion speciation in non-polar solvents: A chemical-separations study. S. Skanthakumar, **L. Soderholm**, M. Piechowicz, S.L. Estes, R. Chiarizia, U. Ruett

9:35 NUCL 47. Structral and spectroscopic studies of U(VI), Np(VI), and Pu(VI) hydrolysis chemistry. **M.G. Autillo**, R. Wilson

10:05 NUCL 48. Counter-cation control of tetravalent actinide hydrolysis and condensation. **S.L. Estes**, L. Soderholm

10:35 Intermission.

10:50 NUCL 49. Complexation of neptunium with small organic ligands using NMR spectroscopy. **C.D. Pilgrim**, H. Mason, M. Zavarin, W.H. Casey

11:20 NUCL 50. Influence of counter-cations on neptunyl speciation and its redox behavior in chloride media. **G. Jin**, S.L. Estes, B. Qiao

TUESDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of Suresh C. Srivastava

C.S. Cutler, *Organizer, Presiding*

1:00 NUCL 51. Advances in radiopharmaceutical chemistry at the BNL Hot Laboratory. **A.B. Packard**

1:45 NUCL 52. Radiometals in diagnostic and therapeutic radiopharmaceutical applications. **S.S. Jurisson**

2:30 NUCL 53. Characterization and *in vivo* evaluation of ^{99m}Tc and ^{188}Re peptides as potential SPECT imaging and radioimmunotherapy agents. **V.A. Sanders**, J.H. Walsh, D. Iskhakov, D. Abdel-Atti, B. Zeglis, J.S. Lewis, K. Czerwinski, L.C. Francesconi

3:15 Intermission.

3:30 NUCL 54. New approach for the isolation of ^{225}Ac isotope from proton irradiated Th target. **A. Younes**, J. Hatcher, H. Cicek, B.P. Burton-Pye, J.M. Fitzsimmons, R.J. Abergel, C.S. Cutler, L.C. Francesconi

4:15 NUCL 55. History of the BNL radioisotope research program: Contributions of Suresh C. Srivastava. **L.F. Mausner**

TUESDAY EVENING

Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

WEDNESDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of Suresh C. Srivastava

C.S. Cutler, *Organizer, Presiding*

8:00 NUCL 56. MU Research Reactor: A valuable resource for medical radioisotopes. **H.M. Hennkens**

8:45 NUCL 57. Manufacturing and applications of Sn-117m in nuclear medicine. **N. Stevenson**

9:30 NUCL 58. Speciation of technetium in ionic liquids. **J. Hatcher**, B.P. Burton-Pye, J.F. Wishart, L.C. Francesconi

10:15 Intermission.

10:30 NUCL 59. Development of novel theranostics. **C.S. Cutler**

11:15 NUCL 60. Award Address (Glenn T. Seaborg Award for Nuclear Chemistry Sponsored by the ACS Division of Nuclear Chemistry and Technology). What it was like to hit upon the "theragnostics" paradigm: "A personal journey" at BNL. **S.C. Srivastava**

12:00 Concluding Remarks.

Radiopharmaceutical Chemistry

Fluorine

Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

WEDNESDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

General Topics in Nuclear Chemistry & Technology

L.C. Francesconi, *Organizer, Presiding*

1:00 NUCL 61. Chelator-free radiolabeling of nanoparticles. **C.M. Drain**, M. Wall, T.M. Shaffer, M. Kircher, J. Grimm

1:15 NUCL 62. EDTA-inspired chelating poly-hydroxamate ligands for lanthanide and actinide coordination chemistry and applications. K. Sockwell, **M. Wetzler**

1:30 NUCL 63. Is ^{210}Po a good indicator for anthropogenic radioactivity? **A. Younes**, C. Alliot, M. Mokili, G. Montavon

1:45 NUCL 64. Luminescent determination of aqueous complexation and extractant kinetics for lanthanide ions. **K. Larsson**, S.P. Mezyk

2:00 Intermission.

2:15 NUCL 65. Application of inelastic neutron scattering for uranium oxyfluorides. **A. Miskowiec**, M.C. Kirkegaard, J. Langford, B. Anderson

2:30 NUCL 66. Structural analysis, complexation, and binding selectivity of lanthanides and actinides: A theoretical investigation. **D.A. Penchoff**, C.C. Peterson, J.D. Auxier, G.K. Schweitzer, R.J. Harrison, H.L. Hall

2:45 NUCL 67. Studies of flerovium homologs with thiacrown ethers. **J.D. Despotopulos**, C.A. Valdez, K.J. Moody, D.A. Shaughnessy

3:00 Intermission.

3:15 NUCL 68. Transport properties of binary and ternary asymmetric warm dense plasma mixtures modeled by orbital-free DFT molecular dynamics. **A. White**, C. Ticknor, J.D. Kress, L. Collins, J. Clerouin, P. Arnault, N. Desbiens

3:30 NUCL 69. *Ab initio* study of the mechanisms and energetics of chlorination on Zr(0001). **E. Kim**, P. Weck, R. Borjas Nevarez, F. Poineau

3:45 NUCL 70. Effect of North Korea's nuclear test in September 2017 for air radiation dose rates inside cabin flights from Singapore to Narita, Japan. **H. Katsura**

4:00 NUCL 71. Development of a microinjection system form high efficiency addition of dopants to the inner surface of National Ignition Facility capsules: ANDARIST. **J.D. Despotopulos**, D.A. Shaughnessy, K.J. Moody, P.M. Grant, C. Cerjan, C.B. Yeamans

4:15 NUCL 72. Technetium incorporation in scheelite: Insights from first-principles. **E. Kim**, M. Ackerman, P. Weck, W. Chernesky, K. Czerwinski

Radiopharmaceutical Chemistry

Carbon-11 & Radionuclide Production

Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

WEDNESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

Computational Methods for Lanthanides & Actinides: Theory & Applications

D.A. Penchoff, *Organizer*

6:00–8:00

NUCL 73. Predicting vibrational spectra of uranyl hydrates. **M.C. Kirkegaard**, A. Miskowiec, A. Shields, B. Anderson

NUCL 74. Coupled cluster studies of intermolecular interactions involving actinide dioxide cations: Cation-cation interactions (CCIs) and complexes with small molecules (CO and N_2). **R. Feng**, K.A. Peterson

NUCL 75. Properties and covalency of high oxidation state AnF_x complexes. **Z. Lee**, M. Vasiliu, A.C. Hartley, J. Kessel, A. Eberly, **D.A. Dixon**

NUCL 76. Active thermochemical tables: A novel approach to understanding actinide chemistry. **S.R. Battey**, D.H. Bross, B. Ruscic, K.A. Peterson

Section A
Ernest N. Morial Convention Center
Hall D

General Topics in Nuclear Chemistry & Technology

L.C. Francesconi, *Organizer*

6:00–8:00

NUCL 77. Continued advancements in the radiochemistry program at the University of Iowa. **T. Forbes**

NUCL 78. New ligands for the selective binding and extraction of light lanthanides. **M.R. Healy**, S. Jansone-Popova, V.S. Bryantsev, B.A. Moyer

NUCL 79. Iodine saturated absorption spectrometer for laser frequency calibration. **S. Pineda**, A. Klose, C. Kujawa, K. Minamisono, N. Everett, R.

‡*Cooperative Cosponsorship*

Powel, D. Garand

NUCL 80. Actinide science at the University of Notre Dame. **A.E. Hixon**

NUCL 81. Synthesis and optical/scintillating properties of transparent ceramics. **R. Balderas**, Y. Mao

NUCL 82. Determination of radioactive krypton (Kr-85) in air. **Y. Ko**, H. Kim, S. Choi, J. Lim, G. Choi, W. Lee

NUCL 83. Determination of radioactivity of uranium and thorium in environmental samples by using fusion and sequential separation method, and its evaluation using key validation parameters. **Y. Ko**, W. Kim, J. Lim, G. Choi, K. Chung, M. Kang, W. Lee

NUCL 84. Investigating the impact of gamma radiation on rare-earth hafnate nanocrystals. **V. Trummel**, M. Pokhrel, D.E. Wall, Y. Mao

NUCL 85. Radiochemistry at Colorado State University. **R. Sudowe**

THURSDAY MORNING

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Computational Methods for Lanthanides & Actinides: Theory & Applications

D.A. Penchoff, *Organizer*
C.C. Peterson, *Presiding*

8:30 Introductory Remarks.

8:45 NUCL 86. Eliminating basis-set incompleteness error in relativistic chemical computations. **R.J. Harrison**

9:15 NUCL 87. Characterization of Es, Fm, Cf separations: A comparison of experimental and computational efforts. **J.D. Auxier**, D.A. Penchoff, M.S. Quint, J. Garrison, H.L. Hall

9:35 Intermission.

9:45 NUCL 88. Composite *ab initio* thermochemistry for f-block elements: Is kcal/mol accuracy achievable? **K.A. Peterson**, D.A. Dixon, S.R. Battey, D. Bross, R. Feng, B. Finney, R. Hermanson, Q. Lu

10:05 NUCL 89. Relativistic *ab initio* accurate minimal basis sets for the lanthanides. **G. Schoendorff**, A.C. West, M.W. Schmidt, K. Ruedenberg, M.S. Gordon

10:25 NUCL 90. Combining minimal basis set localizations with strong correlation approaches towards *ab initio* lanthanide chemistry. **A.C. West**, G. Schoendorff

10:45 Intermission.

10:55 NUCL 91. Understanding structural and thermochemical properties of actinide-containing compounds. **C.C. Peterson**

11:15 NUCL 92. *Ab initio* thermochemistry of transuranium molecules: Halides of U, Np, and Pu. **B. Finney**, K.A. Peterson

11:35 NUCL 93. Understanding the electronic structure and chemical bonding of f-element coordination compounds. **J. Su**, E.R. Batista, P. Yang

11:55 Concluding Remarks.

Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

THURSDAY AFTERNOON

Section A
Embassy Suites New Orleans
Fountainbleu Sec 4

Computational Methods for Lanthanides & Actinides: Theory & Applications

D.A. Penchoff, *Organizer*
C.C. Peterson, *Presiding*

1:30 Introductory Remarks.

1:45 NUCL 94. Local configuration of excess oxygen in UO_{2+x} from the first-principles molecular dynamics. **J. Wang**

2:05 NUCL 95. Crystal structure prediction: Using genetic algorithms and DFT to search for novel stable and metastable uranium oxides. **A. Shields**, A. Miskowiec, B. Anderson

2:25 NUCL 96. Mechanistic models for uranium sorption on iron minerals: Comparing their parametrization and surface species. **F. Bok**, A. Richter, V. Brendler

2:45 Intermission.

2:55 NUCL 97. Electronic structure of uranium arene interactions. **B. Vlaisavljevich**

3:15 NUCL 98. Hydrolysis reactions of actinide oxides and actinide oxides nitrates. **M. Vasiliu**, H. Arnold, K.A. Peterson, J.K. Gibson, D.A. Dixon

3:35 NUCL 99. Computational study of a novel Schiff-base ligand–uranyl complex: Characterization of physical and chemical properties. **A.A. Ridings**, C. Hawkins, T. Yu

3:55 NUCL 100. Structure and bonding of lanthanide hydroxides Ln—OH (Ln=La-Lu). **H. Harb**, L.M. Thompson, H.P. Hratchian

4:15 Concluding Remarks.

Radiopharmaceutical Chemistry
Sponsored by FLUO, Cosponsored by INOR‡, MEDI‡ and NUCL‡

ORGN

Division of Organic Chemistry

R. Broene and S. Silverman, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Encouraging Women into Careers in the Chemical Sciences

(see *WCC*, Tue)

ACS Award in Organometallic Chemistry: Symposium in honor of Clifford P. Kubiak (see INOR, Sun, Mon)

Homogeneous Catalysis for Applied Organic Synthesis (see *CATL*, Mon, Tue)

Recent Advances in Catalytic Carbohydrate Reaction Development (see *CARB*, Tue, Wed)

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Margaret M. Faul

Cosponsored by WCC
K.B. Hansen, *Organizer*
S. Walker, *Presiding*

8:00 ORGN 1. New enantioselective Pauson–Khand-type reactions. **K.M. Brummond**

8:40 ORGN 2. Developing a bioconjugation platform for hybrid modalities. **J.A. Murry**

9:20 ORGN 3. Recent developments in strategies and tactics towards complex secondary metabolites as enabling tools for the study of natural products biology. **E.M. Carreira**

10:00 ORGN 4. Fully continuous multi-step synthesis of drug substance under GMP conditions. **S.A. May**

10:40 ORGN 5. Catalyst-controlled site-selective and enantioselective C-H functionalization. **H.M. Davies**

11:20 Introduction of Awardee.

11:25 ORGN 6. Award Address
(Earle B. Barnes Award for Leadership in Chemical Research Management Sponsored by The Dow Chemical Company Foundation). Perspective on the evolution of process development innovation in the biocentury to enable delivery of novel therapies to patients. **M. Faul**

Section B
Ernest N. Morial Convention Center
R02

Frontiers in Synthetic Organic Photochemistry

Financially supported by Chem (Cell Press), ChemPhotoChem, STREM, Biogen, Boehringer-Ingelheim, ChemComm/ChemSci
T.P. Yoon, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 7. Using light to unlock new enzyme function. **T. Hyster**

8:35 ORGN 8. Decomposition of photocatalytically generated perfluoroaryl radical anions; a powerful synthetic tool for accessing multifluorinated arenes. **J.D. Weaver**

9:05 ORGN 9. Organic transformations via excited state proton transfer. **K. Hanson**, A. Das, S. Ayad, V. Posey

9:35 Intermission.

9:50 ORGN 10. Remote oxo-functionalization of aliphatic amines via photocatalysis. **D.M. Schultz**

10:20 ORGN 11. Chemical synthesis of polycyclobutane-containing natural products. **N.Z. Burns**

Section C
Ernest N. Morial Convention Center
R01

Biologically Related Molecules & Processes

R.D. Broene, *Organizer*
K.J. Clear, *Presiding*

8:00 ORGN 12. Differentiating isomeric glucuronide drug metabolites via gas phase ion/molecule reactions. **Z. Yu**, J. Kong, E. Niyonsaba, M. Easton, X. Ma, R. Yerabolu, D. Ding, H. Zhu, H. Sheng, T. Jarrell, Z. Zhang, H.I. Kenttamaa

8:20 ORGN 13. High affinity fluorescent catecholamine sensor: Applications to monitoring norepinephrine exocytosis. **L. Zhang**, X.A. Liu, K.D. Gillis, T.E. Glass

8:40 ORGN 14. 5-Pyrimidine and 8-purine nucleosides modified with unsubstituted 1,2,3-triazol-4-yl: Synthesis and fluorescent properties. **Z. Wen**, P. Tuttle, A. Vasilyeva, A. Tangar, J. Miksovska, S.F. Wnuk

9:00 ORGN 15. Nanohoops in cells: A new class of cellular imaging agents. **B.M. White**, T.E. Kawashima, R. Jasti

9:20 ORGN 16. Substituted 1-cyanoisoindoles as fluorescent core in the design of labeled strigolactone analogs. **M.A. Van Overtveldt**, T. Heugebaert, C.V. Stevens

9:40 ORGN 17. Heteroditopic receptors for molecular recognition and sensing of anionic lipids. **K.J. Clear**

10:00 ORGN 18. Mechanistic studies on the monoamine oxidase-B catalyzed oxidation of a cyclic tertiary allylamine analog of MPTP using a flavin chemical model. **A. Nakamura**, N. Castagnoli, J. Tanko

10:20 ORGN 19. Visible-light-mediated oxidative demethylation of N^6-methyl adenines. **L. Cheng**

10:40 ORGN 20. Oka fragmentation of the Breslow intermediate is a radical process. **M. McIntosh**

Section D
Ernest N. Morial Convention Center
R04

Asymmetric Reactions & Syntheses

R.D. Broene, *Organizer*
M.B. Tran-Dube, *Presiding*

8:00 ORGN 21. Catalyst controlled diastereoselective reduction of ribonucleosides as PRMT5 inhibitors for the treatment of cancer. **M.B. Tran-Dube**, R. Patman, S.A. Scales, F. Wang, J.F. Braganza, L. Bernier, N. Sach, J. Tatlock, E. Rui, R. Kumpf, M. McTigue, M. Wythes, I.J. McAlpine

8:20 ORGN 22. Enantioselective photoredox catalysis enabled by proton-coupled electron transfer: Development of a concise, asymmetric synthesis of pyrroloindoline alkaloids. **E.C. Gentry**, L.J. Rono, R. Matsuura, M. Hale, R.R. Knowles

‡*Cooperative Cosponsorship*

8:40 ORGN 23. Unprecedented one-pot diasteroselective/asymmetric route for the access of diverse collections of chromeno[4,3-a]pyrrole scaffolds. **T.H. Altel**, S.M. Sieburth

9:00 ORGN 24. Cyclic sulfoximines: Useful building blocks for the expedient synthesis of cyclic sulfinamides and 3-pyrrolines. **J. Ward**, L. Walton, R.A. Stockman

9:20 ORGN 25. Stereodivergent allylation of heteroarylacetates and heteroarylacetamides by synergistic iridium and copper catalysis. **X. Jiang**, J.F. Hartwig

9:40 ORGN 26. Direct Ru(II)-pheox catalyzed asymmetric cyclopropanation of diazomethylphosphonates with *N*-ethylaniline derivatives. **T.T. Le**, S. Chanthamath, K. Shibatomi, S. Iwasa

10:00 ORGN 27. Stereoselective allylic alkylation of β,β-unsaturated β-amino nitriles: Synthetic homoenolate equivalents. **T.B. Wright**, B.W. Turnbull, P. Evans

10:20 ORGN 28. Development of an ideal asymmetric synthesis for BI's 11β-HSD 1 inhibitor. **B. Qu**, X. Wei

Section E
Ernest N. Morial Convention Center
R05

Metal-Mediated Reactions & Syntheses

R.D. Broene, *Organizer*
B.V. Popp, *Presiding*

8:00 ORGN 29. Anionic "ligandless" palladium complexes for cross-coupling catalysis. F. Schroeter, **T. Strassner**

8:20 ORGN 30. Withdrawn

8:40 ORGN 31. Methods to reduce Pd(II) precatalysts to Pd(0) for cross-coupling reactions. **H. Hu**, K.H. Shaughnessy

9:00 ORGN 32. Copper-catalyzed cascade strategy for the synthesis of biologically active tetracyclic isoindolo[1,2-b]quinazolinones and 2-arylquinazolines. **S. Ichake**, C. Yao

9:20 ORGN 33. Revealing the activity of π-acid catalysts using a 7-alkynyl cycloheptatriene. **M. Vayer**, V. Gandon, B. Christophe

9:40 ORGN 34. Discovery of a copper-mediated organoboron aryl Ritter reaction. **A.J. Watson**

10:00 ORGN 35. Free the boronic acids! Allyl- and allenylboronic acids in organic synthesis. **K. Szabo**

10:20 ORGN 36. Synthesis of stereodefined cyclic allylboronic acids and their application on the copper-catalyzed stereoselective coupling with β-diazoketones. **D. Wang**, K. Szabo

10:40 ORGN 37. One regio- and stereoisomeric product in Pd-catalyzed stereospecific couplings of unactivated alkylboronic acids. **J.W. Lehmann**, I.T. Crouch, D.J. Blair, M. Trobe, J. Li, P. Wang, M.D. Burke

11:00 ORGN 38. Catalytic reductive vinylidene transfer reactions. **S. Pal**, Y. Zhou, C. Uyeda

11:20 ORGN 39. *En masse* analysis yields prioritized blocks and bonds for natural product synthesis. **A.M. Palazzolo**, S. Tonddast-Navaei, C.L. Simons, N.T. Russell, J. Peng, J. Skolnick, M.D. Burke

11:40 ORGN 40. Organometallic reductive functionalization reactions of alkenes with CO_2. **B.V. Popp**

Section F
Ernest N. Morial Convention Center
R03

New Reactions & Methodology

R.D. Broene, *Organizer*
A.T. Londregan, *Presiding*

8:00 ORGN 41. Unique reactivity of nitrile-stabilized ammonium ylide as masked C–C=N synthon: An efficient route to access biologically important pyridopyrimidin-4-imines/ones. **M. Saini**, D. Sumkaria, V. Chaudhary, S.K. Guchhait

8:20 ORGN 42. Mild, general and regioselective synthesis of 2-aminopyridines from pyridine *N*-oxides via 2-pyridylpyridinium salts. **A.T. Hoye**, H. Xiong

8:40 ORGN 43. Novel methods for the synthesis of sulfonimidamides: New pharmacophores for the medicinal chemist's toolbox. **F. Izzo**, R. Stockman, U. Luecking

9:00 ORGN 44. New synthetic methods used in the discovery of small molecule PCSK9 inhibitors. **A.T. Londregan**

9:20 ORGN 45. Understanding and interrupting the Fischer azaindolization reaction. **B.J. Simmons**, N.K. Garg

9:40 ORGN 46. Novel method for convenient one-pot two-step synthesis of acylated ureas, carbamates, thiocarbamates and related compounds. **J. Stec**, A. Garcia Hernandez, G. Grooms, A. El-Alfy

10:00 ORGN 47. Synthesis of imines and 1,3-amino alcohols *via* a hydrogen borrowing strategy. **R.E. Whittaker**

10:20 ORGN 48. Cyanide-mediated nitrile-to-nitrile cyclocondensation towards efficient synthesis of polysubstituted pyrroles. **S. Sisodiya**, Y.V. Shah, N. Hura, M. Saini, V. Chaudhary, S.K. Guchhait

10:40 ORGN 49. Asymmetric synthesis of nitrogen heterocycles via iminium ion initiated cyclizations. **M.G. Donahue**

11:00 ORGN 50. Stereoselective synthesis of fused bis-β-lactams by catalytic Mukaiyama Mannich reaction of imines and 2,5-bis(trimethylsilyloxy)furan. **S.W. Laws**, M. Shuyu, B. List, J.T. Shaw

11:20 ORGN 51. Tetrazine-induced release reactions. **R.M. Franzini**, M. Xu, J. Tu

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

Herbert C. Brown Award for Creative Research in Synthetic Methods: Symposium in honor of Gregory C. Fu

Financially supported by Boehringer Ingelheim, STREM
A.R. Howell, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ORGN 52. Molecular surgery via C—H oxidation. **M. White**

1:55 ORGN 53. Turning simplicity into complexity via Ni-catalyzed coupling reactions. **R. Martin**

2:40 ORGN 54. New facets of asymmetric catalysis with helical macromolecular catalysts featuring dynamic chirality. **M. Suginome**

3:25 ORGN 55. Development and applications of selective olefin metathesis catalysts. **R.H. Grubbs**

4:10 ORGN 56. Award Address
(Herbert C. Brown Award for Creative Research in Synthetic Methods Sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment). Nucleophilic substitution reactions: A radical alternative to S_N1 and S_N2 reactions. **G.C. Fu**

Section B
Ernest N. Morial Convention Center
R02

Frontiers in Synthetic Organic Photochemistry

Financially supported by Chem (Cell Press), ChemPhotoChem, STREM, Biogen, Boehringer-Ingelheim, ChemComm/ChemSci
T.P. Yoon, *Organizer, Presiding*

1:20 Introductory Remarks.

1:25 ORGN 57. Synthetic applications of photoredox-mediated ring-opening metathesis polymerization. **A.J. Boydston**

1:55 ORGN 58. Harnessing metal-free photochemistry for synthesis of materials. **J. Read De Alaniz**

2:25 ORGN 59. β C-H functionalization via radical relay chaperones. **D.A. Nagib**

2:55 Intermission.

3:10 ORGN 60. Activating inert bonds via N-centered radicals. **C. Nevado**

3:40 ORGN 61. Photochemical dearomative functionalization with arenophiles. **D. Sarlah**

4:10 ORGN 62. Proton-coupled electron transfer in organic synthesis. **R.R. Knowles**

4:40 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
R01

Biologically Related Molecules & Processes

R.D. Broene, *Organizer*
D. Bandyopadhyay, *Presiding*

1:00 ORGN 63. Modular and diastereoselective bi-directional one-pot routes for the rapid access of constrained collections of b-carbolino-benzoxazepine scaffolds. **T.H. Altel**

1:20 ORGN 64. Exploiting the acinetobactin siderophore system as an antivirulence target in pathogenic *Acinetobacter baumannii*. **J.A. Shapiro**, T.J. Bohac, T.A. Wencewicz

1:40 ORGN 65. Synthetic strategies enabling magnetic isotopes enrichment for parahydrogen based hyperpolarization. **R.V. Shchepin**, N. Chukanov, K. Kovtunov, I. Koptyug, E.Y. Chekmenev

2:00 ORGN 66. Unexpected changes in reactivity arising from fluorine substitution in the synthesis of BACE inhibitors. **M. Mandal**, A. Buevich, H. Wang, R. Mazzola, J.P. Caldwell, J. Cumming, M. Kennedy, P. Orth, A. Brunskill

2:20 ORGN 67. Targeting bacterial drug resistance: Design, synthesis and evaluation of monocyclic 3-amino-1-carboxymethyl-β-lactams as potential inhibitors of Penicillin-binding proteins. **L. Decuyper**, S. Deketelaere, M. Jukič, I. Sosič, E. Sauvage, B. Joris, S. Gobec, M. Dhooghe

2:40 ORGN 68. Synthesis and biological screening of peracetylated glucosyl aurones. **A. Kafle**, S. Handy

3:00 ORGN 69. Synthesis and evaluation of a focused analog library with β-lactam antibiotic potentiation activity in methicillin-resistant *Staphylococcus aureus*. **R. Ulrich**, J. O'Brien, A.J. Wommack, M.S. Blackledge

3:20 ORGN 70. Synthesis and antitumor activity of mimics of the tetrahydrofuran containing acetogenins. **P. Gonzalez**, A. Ramdular, D.R. Mootoo

3:40 ORGN 71. Adventures in carbohydrate chemistry: Acetal-free carbohydrates, and the total synthesis of immunologically active glycolipids. **J.F. Trant**, S. Sadraei, M. Reynolds, E. Igbokwe

4:00 ORGN 72. Synthesis of rocaglate analogues for target identification photoaffinity probes. **N. Vallavoju**, A.B. Beeler, J.A. Porco

4:20 ORGN 73. Heme carbene reacts differently from native heme enzymes in C-H functionalization. R. Khade, **Y. Zhang**

4:40 ORGN 74. Discovery of new bioactive small molecules and approaches at new chemical screening libraries. **R. Rafferty**

Section D
Ernest N. Morial Convention Center
R04

Asymmetric Reactions & Syntheses

‡*Cooperative Cosponsorship*

R.D. Broene, *Organizer*
J.L. Bolliger, *Presiding*

1:00 ORGN 75. Enantioselective total synthesis of polychlorinated natural products. **G. McKenna**, M.L. Landry, N.Z. Burns

1:20 ORGN 76. Synthesis of sesquiterpene-tropolones. **C.Y. Bemis**, C. Ungarean, D. Sarlah

1:40 ORGN 77. Asymmetric synthesis of trifluoromethyl-substituted cyclopropanes via myoglobin-catalyzed transfer of trifluoromethylcarbene. **A. Tinoco**, R. Fasan

2:00 ORGN 78. Synthesis enabled design of new GPR40 full agonists: A collaborative approach between process and medicinal chemistry. **R. Orr**

2:20 ORGN 79. Total synthesis of baulamycins A & B. **A. Steele**, G. Ernouf, Y. Eun Lee, W. Wuest

2:40 ORGN 80. Synthesis of unsymmetrical perylene tetracarboxylic derivatives with liquid crystalline phase. **X. Zhao**

3:00 ORGN 81. High enantioselective aldol reaction catalyzed by a one-handed helical poly(phenylacetylene) bearing L-hydroxyproline pendants in aqueous solvent. **C. Zhang**, S. Bo, Y. Qiu, F. Wang, Y. Wang, T. Satoh

3:20 ORGN 82. DCC: A modular approach to bifunctional organocatalysts. **J.L. Bolliger**, L. Ardon Munoz

Section E
Ernest N. Morial Convention Center
R05

Metal-Mediated Reactions & Syntheses

R.D. Broene, *Organizer*
J.R. Green, *Presiding*

1:00 ORGN 83. TMS-protected alkynes as selective cross coupling partners in Ti catalyzed [2+2+1] pyrrole synthesis. **H. Chiu**, I. Tonks

1:20 ORGN 84. Molybdenum salan complexes as catalysts for deoxydehydration of vicinal diols. **N.J. Wagner**, A. John, S. Gibbons-Stovall, C. Navarro

1:40 ORGN 85. Tungsten-promoted dearomatization of benzene: A regio and stereoselective route to functionalized cyclohexenes. **K. Wilson**, J. Smith, W. Harman

2:00 ORGN 86. Iron-catalyzed synthesis of cyclopropanes by *in-situ* generation and decomposition of electron-rich diazo compounds. **E.M. Allouche**, A. Al-Saleh, A.B. Charette

2:20 ORGN 87. Intermediates and reactivity in iron-catalyzed cross-couplings of alkynyl Grignard reagents with alkyl halides. **J.L. Kneebone**, W.W. Brennessel, M.L. Neidig

2:40 ORGN 88. Highly efficient removal of water soluble NHC-Ru catalyst by host-guest interaction. **C. Kim**, H. Chung

3:00 ORGN 89. Ruthenium-catalyzed C–H hydroxylation of amines: Reaction development and mechanistic considerations. **J. Mack**, J. Du Bois, M.S. Sigman

3:20 ORGN 90. Alkynedicobalt mediated vinylogous Nazarov reactions. S. Almubayedh, **J.R. Green**

3:40 ORGN 91. Application of a chiral binaphthyl-based scaffold for dirhodium(II) biscarboxylate ligand with β-quaternary carbon centers. **P. Chen**, K. Setthakarn, J. May

4:00 ORGN 92. Leveraging metal-carbenes for assembling complexity. **I. Sharma**

4:20 ORGN 93. Catalytic use of low-valent cationic gallium(I) complexes π-acids. **B. Christophe**

Section F
Ernest N. Morial Convention Center
R03

New Reactions & Methodology

R.D. Broene, *Organizer*
A. Bugarin, *Presiding*

1:00 ORGN 94. Withdrawn

1:20 ORGN 95. Enantioselective Au(III) catalysis. **P. Bohan**, D. Toste

1:40 ORGN 96. Interrupted, aerobic oxidative Heck reaction involving selective C–C bond scission for synthesis of 1,3-dienes and polyenes. **N. McAlpine**, L. Wang, B. Carrow

2:00 ORGN 97. Cobalt-catalyzed carbonylative cross-coupling of alkyl tosylates and dienes: Stereospecific synthesis of dienones at low pressure. **B.T. Sargent**, E.J. Alexanian

2:20 ORGN 98. Regioselective Simmons-Smith type cyclopropanations of polyalkenes under catalyst control. **J. Werth**, C. Uyeda

2:40 ORGN 99. Nickel catalyzed intermolecular, three-component carboacylation of alkenes via amide C-N bond activation. **A.A. Kadam**, L.M. Stanley

3:00 ORGN 100. Formal β-C–H functionalization of amines by Pd catalyzed allylation of 2-azaallyl anions generated from amines and a quinone. **L.M. Mori Quiroz**, S.S. Londhe, M.D. Clift

3:20 ORGN 101. Development of unique functional group interconversions. **A. Bugarin**

3:40 ORGN 102. Transforming primary benzylic amines into di(hetero) arylmethanes: Nickel-catalyzed Suzuki–Miyaura cross-couplings of benzylic amine derivatives via C–N bond activation. **J. Liao**, W. Guan, J. Tomlin, M. Garnsey, M.P. Watson

4:00 ORGN 103. Negishi alkylation of alkyl pyridinium salts: Alkyl-alkyl cross-couplings via C–N bond activation of alkyl amine derivatives. **S. Plunkett**, C. Basch, S.O. Santana, M.P. Watson

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

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SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

Asymmetric Reactions & Syntheses

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 104. Withdrawn

ORGN 105. Catalytic enantioselective phosphorylation of an FTY720 model diol. **E. Ouellette**, B.R. Sculimbrene

ORGN 106. Improved stereoselectivity in the synthesis of cylopropyl peptidomimetics using quinine-based catalysts. N.K. Dunlap, **T.J. Orr**

ORGN 107. Biocatalysis: Investigating the reaction profile of promiscuous amine dehydrogenases. **K. Smith**, **S. Davenport**, **A. Vargas**, B. Bommarius, A.S. Bommarius, **B.D. Feske**

ORGN 108. Synthesis of enamine resistant substrates for an amine dehydrogenase library. **A. Vargas**, **S.M. Johnston**, **P. Nguyen**, B. Bommarius, A.S. Bommarius, **B.D. Feske**

ORGN 109. Preparation of chiral aziridines through a copper-catalyzed asymmetric reduction of 2*H*-azirines. **R. Turro**, T. Weigel, J. Unger

ORGN 110. Biocatalytic asymmetric reduction of substituted 2-tetralones. **M.M. Musa**, O. Bsharat, M. Takahashi, S.M. Hamdan, C. Vieille, S.A. Oladepo

ORGN 111. Computational investigation on the facial selectivity and eanantioselectivity of oxyallyl cation catalysis. **C.Q. He**, P. Yu, C. Lam, K.N. Houk

ORGN 112. Rhodium-catalyzed enantioselective [4+2] cycloadditions of vinylcarbenes with dienes. **B. Zhang**, H.M. Davies

ORGN 113. Combined DFT and experimental study of the base and acid catalyzed *oxa*-Michael reaction in THP synthesis: Reinterpretation of the selectivity-determining factors. **D. Csokas**, R.O. Ramabhadran, A. Ho, R.W. Bates

ORGN 114. Asymmetric catalyzed cycloaddition via copper-allenylidene process for preparation of tetrahydroquinolines fused with δ-lactone moiety. H. Chen, X. Lu, X. Xia, **X. Wu**

ORGN 115. Synthesis of chiral heterocyclic compounds from enantiomerically rich sulfa-Michael adducts. **D. Tözendemir**, C. Tanyeli

ORGN 116. Synthesis and evaluation of new imidazolidinone catalysts for the alpha-sulfamidation of aldehydes. T. Broerman, D.L. Martinec, S.A. Lowe, **T.C. Coombs**

ORGN 117. Asymmetric [3+2] cycloadditions of azomethine ylides generated from chiral sulfinamide precursors. **D. O'Connor**, R. Stockman

ORGN 118. Development of a dynamic kinetic resolution of aryl-naphthoquinone atropisomers via a cinchona alkaloid catalyzed nucleophilc addition of thiophenols. S.M. Maddox, **G.A. Dawson**, J. Gustafson

ORGN 119. Asymmetric organocatalytic addition of β-azido ketones to isatin-derived ketimines. **S. Karahan**, C. Tanyeli

ORGN 120. Preparation of 3-*endo*-benzylisobornylamine and related compounds. **A.J. Dahl**, **C.J. Hartwick**, D.E. Lewis

ORGN 121. Synergistic catalysis: A novel approach to enantioselective reactions. **W. Bio-Sawe**, H. Subramanian, M.P. Sibi

ORGN 122. Expanding the Felkin-Anh model: A study of the stereoselectivity of imines. **B. Rich**, L.C. Moore, A. Lo, J.T. Shaw

ORGN 123. Atroposelective dynamic kinetic resolution of diaryl ether naphthoquinones through alkylation. **A.N. Dinh**, R. Noorbehesht, **A. Jackson**, J. Gustafson

ORGN 124. Accessible path to forming a range of asymmetric rhodamine derivatives. C.J. Stephenson, **L.V. Odom**, **V. Cinnater**, **K. Cleveland**, D. Rich, M. Bollinger

ORGN 125. Withdrawn

ORGN 126. Carboxylic acid activation: Investigation of an enantioselective iodolactonization of 1,4-cyclohexadienes. **H. Lee**, M.T. Knowe, J.N. Johnston

ORGN 127. Peptoid catalysts for the enantioselective trifluoromethylation of carbonyls. **S. DeCarlo**, B.C. Gorske

Section A
Ernest N. Morial Convention Center
Hall D

CH Activation

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 128. Copper-catalyzed intramolecular oxidative C(sp^3)–H functionalization for the synthesis of heteroaromatics. **K. Nozawa-Kumada**, S. Saga, S. Kurosu, Y. Kondo

ORGN 129. Stereoselective 3-component catalytic addition of C–H bonds to C=C and polarized π-bonds. **J.A. Boerth**, J. Hummel, J.A. Ellman

ORGN 130. Platinum catalyzed double acylation of 2-(aryloxy)pyridines via direct C-H activation. **E. Javed**, **S. Huo**, D. McAteer, L. Huo

ORGN 131. Directed Cp*Rh(III)-catalyzed fluorosulfonylvinylation of arenes. **M.P. Huestis**

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ORGN 132. Allylic C–H etherification and esterification of 1,2-trans-disubstituted olefins. **T. Farmer**, S. Blakey

ORGN 133. Development of Rh(III) Cp* catalyzed allylic C–H amination via π-allyl intermediates. **J.S. Burman**, S. Blakey

ORGN 134. Tunable differentiation of tertiary C–H bonds in intramolecular transition metal-catalyzed nitrene transfer reactions. **J.R. Corbin**, J.M. Schomaker

ORGN 135. Mechanistic studies of Rh(III) catalyzed allylic C–H amination. **D.C. Salgueiro**, S. Blakey, R.J. Harris

ORGN 136. Withdrawn

ORGN 137. Cyanoborylation and nitrile-directed C-H activation as a versatile combined approach to C-H functionalization. **A.Q. Ansel**, W. Zhao, J. Montgomery

ORGN 138. Synthesis of unsymmetrical 2,6-diarylaniline derivatives. **S. Kwak**, O. Daugulis

ORGN 139. Directing group assisted C-H amidation of arenes. **K. Das**, P. Kilaru, P. Zhao

ORGN 140. N-heterocyles synthesis via C-H functionalization using transition metal. **S. Acharya**

Section A
Ernest N. Morial Convention Center
Hall D

Metal-Mediated Reactions & Syntheses

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 141. Development of a practical and scalable synthesis of a Glucokinase activator. **Y. Yamashita**, Y. Morinaga, M. Kasai, T. Hashimoto, Y. Takahama, A. Ohigashi, S. Yonishi, M. Akazome

ORGN 142. Cyclization using alkene and acylphosphonate under Co catalysis. **H. Hori**, S. Arai, A. Nishida

ORGN 143. Formal aromaticity-transfer for palladium-catalyzed coupling between phenols and pyrrolidines/indolines. **Z. Qiu**, J. Li, C. Li

ORGN 144. Organocopper reagents that behave as functionalized acyl anions. **G.W. Ebert**, J. Ebert

ORGN 145. Synthesis and catalytic application of asymmetrically substituted 1,3-diphosphines. **B.R. Headford**, K.H. Shaughnessy

ORGN 146. Withdrawn

ORGN 147. Conversion of primary amines to symmetrical secondary and tertiary amines using a Co-Rh heterobimetallic nanocatalyst. **Y.K. Chung**, H. Chung

ORGN 148. Platinum-graphene catalyst for the solventless hydrosilylation of olefins. **C. Kong**, S. Gilliland, B. Clark, F. Gupton

ORGN 149. Exploring axial coordination of ligands in dirhodium (II) paddlewheel complexes in Si-H insertion reactions. **W. Sheffield**, A. Darko

ORGN 150. Palladium-catalyzed carbonylative cross-coupling reaction between aryl(heteroaryl) iodides and tricyclopropylbismuth: Expedient access to aryl cyclopropylketones. **E. Benoit**, J. Dansereau, A. Gagnon

ORGN 151. Mechanistic investigations of the copper-catalyzed stereoselective cross-coupling of cyclic allylboronic acids with δ-diazoketones. **D. Wang**, K. Szabo

ORGN 152. C–H functionalization via lithium amide zincate base-mediated deprotonative zincation. **K. Bitting**, Q. Wang

ORGN 153. Divergent transmetalation to palladium from boron vs. tin reagent. **S. Shreiber**, J. Russell, S.R. Neufeldt

ORGN 154. Recent advantages in gold I/III catalyzed alkyne activations. **S. Zhang**, J. Wang, X. Shi

ORGN 155. Radical-ionic and ionic-radical functionalizations of cobalt-complexed acetylenic bis-ethers. **S. Gershelis**, G.G. Melikyan

ORGN 156. Allylic triad as a dichotomous reaction site in cobalt-mediated radical transformations of 1,4-enynes. **S. Guarina**, G.G. Melikyan

ORGN 157. Carbon-carbon bond formation in intramolecular setting: Cobalt-mediated stereoselective synthesis of cyclohexanes and tetralins. **E.Y. Artashyan**, **M.K. Parunyan**, G.G. Melikyan

ORGN 158. Spectroscopic characterization of diiodomethylzinc iodide: Application to the stereoselective synthesis and functionalization of iodocyclopropanes. **E.M. Allouche**, S. Taillemaud, A.B. Charette

ORGN 159. Synthesis of cyclic conjugated diyne through gold-catalyzed alkyne oxidative coupling. **C. Wei**, **X. Shi**

ORGN 160. Nicholas reactions of organotrifluoroborates. **B. St. Onge**, J. Battersby, J.R. Green

ORGN 161. Carbon-Carbon bond forming reactions medaited by gold(I/III) redox events. **S. Kim**, D. Toste

ORGN 162. Metal-mediated synthesis of 2-amino free-reducing sugars as glycodiversification building blocks. **V. Huang**, **J. Lam**, C.M. Rojas

ORGN 163. Stabilization of dirhodium paddlewheel carbenoids through tethered axial coordination. **D. Cressy**, K.B. Idrees, L. Lopez, A. Darko

ORGN 164. Molybdenum-catalyzed regioselective synthesis of 3-substituted indoles. **N. Ummidisetti**, R. Srivastava

ORGN 165. Highly diastereoselective (E)-trisubstituted alkenes containg cyclopropyl and trimethylsilyl methyl moities via organoboranes. **N.G. Bhat**

ORGN 166. Peri-coupling of organometallic reagents for the synthesis of perylenes and oligorylenes. **I. Perry**, J. Rawson, L. Holt, J. Markiewicz

ORGN 167. Highly daistereoselective synthesis of (*Z*)-trisubstituted alkenes containing trimethylgermyl and (1,3-dioxan-2ylethyl) moieties via organoboranes. **N.G. Bhat**

ORGN 168. Controlled Kumada catalyst-transfer polymerization of a fluorinated donor-acceptor conjugated monomer. **C. Roselli**, P.R. Payne, M. Brookhart, W. You, M.R. Gagne

ORGN 169. Synthesis and characterization of *beta-* and *meso-*functionalized carbohydrate-porphyrin conjugates (CPC's). **M.C. Bennion**, D. Dennis, M. Burch, A. Henderson, M.R. Parris, N. Abualeinan, L. Russel, **N.L. Snyder**, **J.V. Ruppel**

ORGN 170. Boracarboxylation of vinyl arenes with redox-neutral copper catalysis: Expanding substrate and boron reagent scope and improving catalyst efficiency. **S. Knowlden**, **T.M. Perrone**, A. Gregory, N. Ziemer, B.V. Popp

ORGN 171. Novel decarboxylative C-C bond formation via metallaphotoredox catalysis. **T. Wang**, J. Kautzky, R.W. Evans, D.W. MacMillan

ORGN 172. Enantioselective allylic amination using a heterobimetallic catalyst. **C. Ence**

ORGN 173. Catalyst-dependent hydroazidation of 5-ethynyl pyrimidine nucleosides: Formation of vinyl azides *versus* triazoles. **P. Tuttle**, Z. Wen, A. Vasilyeva, S.F. Wnuk

ORGN 174. Efficient hydroformylation of 1,1,3-trisubstituted allenes. **J. Eshon**

ORGN 175. Two-step derivatization of fluconazole via radical fragmentation of a Breslow-type intermediate. **J. Kubik**, J. Rivero, C. Canote, J. Sonnentag, D. McNabb, J. Avery, M. McIntosh

ORGN 176. Withdrawn

ORGN 177. Synthesis and coordination of various phenylisocyanide ligands to a cobalt precatayst for dimerization of linear alpha olefins. R.D. Broene, **J.H. Morris**

ORGN 178. Thienopyrroledione-based photosensitizers for high voltage dye-sensitized solar cells. **A. Peddapuram**

Section A
Ernest N. Morial Convention Center
Hall D

Photoredox Chemistry

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 179. Withdrawn

ORGN 180. Catalytic Birch reduction via photocatalytic C-F functionalization: An alternative approach to multifuorinated arenes. **M. Khaled**, J. Day, J.D. Weaver

ORGN 181. Formal Giese addition of C-H nucleophiles enabled by visible light mediated triplet catalysis. **G. Lee**, S. Hong

ORGN 182. Photo-induced transition metal catalyzed regio- and E/Z- selective hydroalkylation of activated alkynes. **S. Go**, G. Lee, S. Hong

ORGN 183. New cross coupling reactions of alkyl halides. **D.J. Kornfilt**, D.W. MacMillan

ORGN 184. Photoredox-catalyzed isotopic labeling of pharmaceutical compounds. **Y. Loh**, K. Nagao, A. Hoover, D. Hesk, N. Rivera, S.L. Colletti, I. Davies, D.W. MacMillan

ORGN 185. Withdrawn

ORGN 186. Revisiting metallaphotoredox cross electrophile coupling for the construction of challenging C-C bonds. **S. Cardinal**, D.W. MacMillan

ORGN 187. Visible-light mediated C-F bond formation. **G. Lovett**, D.W. MacMillan

ORGN 188. Selective sp^3 C–H alkylation via polarity-match-based cross-coupling. C. Le, **Y. Liang**, R.W. Evans, X. Li, D.W. MacMillan

ORGN 189. Metallaphotoredox catalysis for the construction of synthetically important C-C bonds. **V. Bacauanu**, M. Kondo, D. Fernandez, D.W. MacMillan

ORGN 190. New C-C and C-X bond forming reactions enabled by photoredox catalysis. **P. Viereck**, D.W. MacMillan

ORGN 191. Withdrawn

ORGN 192. C-N bond formation via the merger of photocatalysis and base metal catalysis. **J. Mohr**, D.W. MacMillan

ORGN 193. Selective hydrogen atom abstractuon via the induction of hydricity: The direct β-arylation of alcohols via photoredox, HAT and nickel catalysis. **J. Twilton**, M. Christensen, D. DiRocco, R. Ruck, I.W. Davies, D.W. MacMillan

ORGN 194. Photoredox-catalyzed β-amino C–H bond functionalization. **K. Nagao**, Y. Loh, A. Hoover, D. Hesk, N. Rivera, S.L. Colletti, I. Davies, D.W. MacMillan

ORGN 195. Direct aldehyde C–H arylation and alkylation via metallaphotoredox catalysis. **X. Zhang**, D.W. MacMillan

ORGN 196. Metallaphotoredox catalysis for novel C-C bond formation. **P.J. Sarver**

ORGN 197. Metal-free visible light C–H alkylation of heteroarenes using hypervalent iodine dicarboxylates. **J. Genovino**, Y. Lian, Y. Zhang

ORGN 198. Metallaphotoredox-catalysed cross-coupling of carboxylic acids with alkyl halides. **R. Smith**, C. Johnston, S. Allmendinger, D.W. MacMillan

ORGN 199. Photoinduced oxidative cyclization reactions for the preparation of complex ring systems. **C. Taylor**, A. Alshreimi, P. De Lijser

ORGN 200. Metallaphotoredox catalysis for the synthesis of unnatural amino acids. **T. Faraggi**, C. Rouget-Virbel, D.W. MacMillan

ORGN 201. Withdrawn

ORGN 202. Metallaphotoredox-mediated synthesis of unnatural

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phenylalanines. **C.A. Rouget Virbel**, T. Faraggi, D.W. MacMillan

ORGN 203. Isotopic labeling enabled by metallaphotoredox catalysis. **R. Pipal**, S. Ren, P. Zhang, D. Hesk, I. Davies, D.W. MacMillan

ORGN 204. Application of photoisomerization for the synthesis of enantioenriched b-aryloxyesters. **E. Swift**, S. Shekhar

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

Twenty Years of Organo- & Photoredox Catalysis

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of David W.C. MacMillan

S.M. Silverman, *Organizer*
R.R. Knowles, *Presiding*

8:00 Introductory Remarks.

8:05 ORGN 205. Design of catalysts using pentacarboxycyclopentadienes (PCCPs). **T.H. Lambert**

8:30 ORGN 206. A few of my favorite rings: Catalysis inspired by cyclic structures. **V.M. Dong**

8:55 ORGN 207. Importance of long-range electrostatics in drug discovery: Discovery of selective SYK/Zap70 dual inhibitor MK-8457 for the treatment of rheumatoid arthritis. **A. Northrup**

9:20 ORGN 208. C-H and C-O functionalization via radical chaperones. **D.A. Nagib**

9:45 ORGN 209. Development of new reactions using radical anion intermediates. **N. Jui**

10:10 ORGN 210. Dual catalysis strategies for site selective functionalization of azaheterocycles. **J. Van Humbeck**

10:35 ORGN 211. Selective functionalization of pyridines and diazines via heterocyclic phosphonium salts. **A. McNally**

11:00 Introduction of Awardee.
11:05 ORGN 212. Award Address (Gabor A. Somorjai Award for Creative Research in Catalysis Sponsored by the Gabor A. and Judith K. Somorjai Endowment Fund). New photoredox reactions. **D.W. MacMillan**

Section B
Ernest N. Morial Convention Center
R02

Successful Products & Models of Undergraduate-Based Research: Good Science, Better Scientists

Financially supported by Denison University, Bruker AXS, Inc.
J.J. Reczek, K.A. Wheeler, *Organizers, Presiding*

8:20 Introductory Remarks.

8:25 ORGN 213. Synthesis, analysis, and devices: Designing diversity of appeal in organic materials research with undergraduates. **J.J. Reczek**

8:50 ORGN 214. Adventures in undergraduate research: The development of glowing polymers for disease detection. **C.B. Cooley**

9:15 ORGN 215. Intramolecular chiral relay at stereogenic nitrogen: The design, synthesis, and application of oxadiazinones as chiral auxiliaries: Perspective in conducting research at an institution that offers a BS and MS degree in chemistry. **S.R. Hitchcock**

9:40 ORGN 216. Case studies in solid-state chemistry from undergraduate students in the pharmaceutical industry. **M.B. Hickey**

10:05 Intermission.

10:20 ORGN 217. Pi-expanded coumarin crankshafts and propellers as aryl-aryl molecular geometry switches. **B.J. Dahl**

10:45 ORGN 218. Better life, better science: Intern/co-op program in pharmaceutical development at biogen. M.L. Peterson, **J. Xu**, K. Vasudevan

11:10 ORGN 219. Importance of effective mentoring in undergraduate research in organic chemistry. **K.M. Morgan**, K.E. Johanson, M. Foroozesh, T.S. Coston

11:35 ORGN 220. Lewis acid mediated activation of aryl and alkyl sulfonyl fluorides towards sulfonamides. **N.D. Ball**, C.P. Woroch, M. Rusznak, L. Cleary, P. Mukherjee, C. am Ende, M.R. Reese, J.W. Tucker, J.M. Humphrey, R.W. Franzese, S.M. Etuk, S.C. Kwan

Section C
Ernest N. Morial Convention Center
R01

Biologically Related Molecules & Processes

R.D. Broene, *Organizer*
S. Choi, *Presiding*

8:00 ORGN 221. New zampanolide mimic with a stable side chain: Synthesis and antiproliferative evaluation. **Q. Chen**, G. Chen, R. Wang, B. Vue, M. Gonzalez

8:20 ORGN 222. Biophysical basis for the high-affinity binding of a vancomycin-resistant cell wall peptide by oritavancin. S. Bowden, S. Tang, C. Josepth, **S. Choi**

8:40 ORGN 223. Development of small molecule therapeutics for the resurrection and reactivation of acetylcholinesterase. **A.J. Franjesevic**, Q. Zhuang, B. Scarpitti, J. Tabbaa, S. Davis, N. Rigel, C. Watt, C.S. Callam, C.M. Hadad

9:00 ORGN 224. Reaction-based chemiluminescent probe for peroxynitrite detection in living cells. **J. Cao**, A.R. Lippert

9:20 ORGN 225. Ester- and amide-based MultiQACs: Multicationic soft antimicrobial agents. **R. Allen**, M. Jennings, M. Mitchell, S. Al-Khalifa, W. Wuest, K.P. Minbiole

9:40 ORGN 226. Development of ligands for serotonin 2A and 2C receptors. **Y. Yang**

10:00 ORGN 227. Strain-promoted double-click functionalised stapled peptides for inhibiting protein-protein interactions. **K. Sharma**, D.R. Spring

10:20 ORGN 228. Second generation oxoeicosanoid receptor antagonists: Increased potency and improved pharmacokinetics. **S. Chourey**, Q. Ye, C. Reddy, R. Wang, S. Gravel, C. Cossette, I. Slobodchikova, **D. Vuckovic**, **W.S. Powell**, J. Rokach

10:40 ORGN 229. Parabens find utility in more than just everyday products. **A.A. Yeagley**

11:00 ORGN 230. Hydrogen bonding with fluorine. **J.I. Day**, J.D. Weaver

11:20 ORGN 231. Protection of the benzoxaborole functionality: Synthesis and functionalization of zwitterionic benzoxaborole complexes. **J. Gamrat**, G. Mancini, S. Burke, J.W. Tomsho

11:40 ORGN 232. Glycofullerenes: Synthetic strategies for inhibiting *Ebola* virus infection. **N. Martin**

Section D
Ernest N. Morial Convention Center
R04

Asymmetric Reactions & Syntheses

R.D. Broene, *Organizer*
M. McIntosh, *Presiding*

9:00 ORGN 233. Enantioselective synthesis of allylic fluorides via iridium-catalyzed dynamic kinetic asymmetric transformations of racemic allylic trichloroacetimidates with $Et_3N{\cdot}3HF$. **A. Sorlin**, J. Mixdorf, H.M. Nguyen

9:20 ORGN 234. Enhanced catalyst system from copper and silanediols. Y. Guan, **J. Attard**, A. Mattson

9:40 ORGN 235. Recent advance on enantioselective synthesis of allenes. **S. Ma**

10:00 ORGN 236. Asymmetric β-arylation of amino acids. **D.J. Leonard**, J. Ward, J. Clayden

10:20 ORGN 237. Enantioselective catalysis with a unique silanediol and copper combination. **Y. Guan**, J. Attard, A. Mattson

10:40 ORGN 238. Development of a nucleophilic dynamic kinetic resolution of aryl-naphthoquinone atropisomers. **S.M. Maddox**, G.A. Dawson, J. Gustafson

11:00 ORGN 239. Enantioselective hydration of aminonitriles mediated by aldose sugars. **A.J. Wagner**, D.Y. Zubarev, A. Aspuru-Guzik, D.G. Blackmond

11:20 ORGN 240. Medium-sized heterocycles: Stereoselective synthesis and their unique transformations. **Y. Zhao**

Section E
Ernest N. Morial Convention Center
R05

Materials, Devices & Switches

R.D. Broene, *Organizer*
S.C. Blackstock, *Presiding*

8:40 ORGN 241. Understanding perturbations to mechanochemical reaction paths for the engineering of force-responsive materials. **A. Kelly**, P.M. Zimmerman

9:00 ORGN 242. Optically reconfigurable charge-transfer liquid crystals. M. Van Winkle, D.A. Scrymgeour, **B. Kaehr**, J.J. Reczek

9:20 ORGN 243. Benzyalkylsilane molecular rectifiers with electron donating and electron withdrawing terminal groups. **A.D. Broadnax**, Z.A. Lamport, A. DelaCourt, B. Scharmann, O.D. Jurcheschu, M.E. Welker

9:40 ORGN 244. Designed nanotubes formed by the dynamic assembly of imine-linked macrocycles. **A. Chavez**, C. Sun, M. Shen, M. Olvera De La Cruz, W. Dichtel

10:00 ORGN 245. Optics-free, non-contact microfluidics with graphene nano-island strain sensors. **C. Dhong**, S.J. Edmunds, D.J. Lipomi

10:20 ORGN 246. Graphene nanoribbon superstructures: Strategies for massive absorptivity. **S. Peurifoy**

10:40 ORGN 247. Redox-assisted self-assembly of π-conjugated chromophores provides function-enhanced superstructures. **O. Jean-Hubert**, K. Liu, A. Levy, C. Liu

11:00 ORGN 248. Photo-electro responsive materials using redox auxiliary catalysis. **S.C. Blackstock**

11:20 ORGN 249. Enhancing catalytic turnover in the redox auxiliary mediated *Z—>E* azobenzene switching. **D. Warner**, S.C. Blackstock

Section F
Ernest N. Morial Convention Center
R03

New Reactions & Methodology

R.D. Broene, *Organizer*
P.A. Vadola, *Presiding*

8:20 ORGN 250. Aryne reactions with element-element sigma bonds. **M. Mesgar**, J. Nguyen-Le, O. Daugulis

8:40 ORGN 251. Lewis base activation of benzyl boronic acid pinacol ester for nucleophilic additions. **T.J. Barker**, M.R. Hollerbach

9:00 ORGN 252. Homoconjugate addition of organoboron nucleophiles to activated cyclopropanes. **T.N. Nguyen**, J. May

9:20 ORGN 253. Harnessing the reactivity of strained allene intermediates. **J. Barber**, N.K. Garg

9:40 ORGN 254. Dearomative spirocyclization of *N*-aryl alkynamides for the synthesis of spirolactams. **P.A. Vadola**, T.L. Vacala, P.R. Carlson, A. Arreola-Hester, E.W. Makhoul, C.G. Williams

10:00 ORGN 255. Mild and environmentally benign reactivity of a novel, highly concentrated, organic HCl reagent for 1,2-alkene difunctionalization. **R. Ebule**, G.B. Hammond, B. Xu

‡*Cooperative Cosponsorship*

10:20 ORGN 256. Application of the enyne Cope rearrangement in terpenoid natural product synthesis. **S. Scott**, A.J. Grenning

10:40 ORGN 257. Amino ketones from alkenes & amides by electronic control of the Kulinkovich-de Meijere reaction. B.P. Derstine, P.B. Finn, **S.M. Sieburth**

11:00 ORGN 258. Development of novel benzyloxymethyl protecting groups and their application to the stereoselective glycosylation. **K. Torikai**, T. Sato, Y. Joh, M. Karak, T. Oishi, M. Suenaga

11:20 ORGN 259. Novel multicomponent reaction chemistries from the Domling laboratory. **A. Doemling**

11:40 ORGN 260. Non-scorpionate tris(pyrazolyl)methane and related ligands via the reaction of 3-amino- or 3-hydroxypyrazole with aldehydes and ketones. **B.M. Ahmed**, N. Rudell, I. Soto, G. Mezei

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

ACS Award for Affordable Green Chemistry: Symposium in honor of B. Frank Gupton & D. Tyler McQuade

R.E. Maleczka, *Organizer*
A. Longstreet, *Presiding*

1:00 ORGN 261. On being green: Can flow chemistry help? **S. Ley**

1:30 ORGN 262. Use of continuous flow technology for the synthesis of active pharmaceutical ingredients. **C. Kappe**

2:00 ORGN 263. Development of scalable and cost-effective API synthesis through chemical innovation. **C.H. Senanayake**

2:30 ORGN 264. Flow hydrogenation of pharmaceutical intermediates. **J. Hawkins**

3:00 ORGN 265. Modular assembly systems for the production of affordable medications in continuous flow. **P.H. Seeberger**

3:30 ORGN 266. Chemistry: Throwing a curve in the value chain. **J.B. Manley**

4:00 ORGN 267. Award Address (ACS Award for Affordable Green Chemistry Sponsored by The Dow Chemical Company and endowed by Rohm and Haas Company). Realizing efficient synthesis of critical medicines by combining mechanistic organic chemistry and continuous methods. **D.T. Mc Quade**

4:30 ORGN 268. Award Address (ACS Award for Affordable Green Chemistry Sponsored by The Dow Chemical Company and endowed by Rohm and Haas Company). Access to global healthcare through process intensification of active pharmaceutical ingredients. **F. Gupton**

Section B
Ernest N. Morial Convention Center
R02

James Flack Norris Award in Physical Organic Chemistry: Symposium in honor of Cynthia J. Burrows

Cosponsored by WCC
M.K. Boyd, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 269. Expanded porphyrins: Adventures in aromaticity, antiaromaticity, and semi-aromaticity. **J.L. Sessler**

1:40 ORGN 270. Synthetic chiral carbon nanoforms. **N. Martin**

2:15 ORGN 271. Developing modern physical organic analysis tools. **M.S. Sigman**

2:50 ORGN 272. Mechanistic studies on DNA damage. **M.M. Greenberg**

3:25 ORGN 273. DNA repair, organic chemistry & cancer: It's all about the base. **S.S. David**

4:00 ORGN 274. Award Address (James Flack Norris Award in Physical Organic Chemistry Sponsored by the ACS Northeastern Section). Physical organic chemistry on the genome. **C.J. Burrows**

Section C
Ernest N. Morial Convention Center
R01

At the Frontier of Stereoselective Alkene Halofunctionalization
Cosponsored by ORGN
Financially supported by Thieme
J.N. Johnston, *Organizer, Presiding*

1:00 ORGN 275. Amino difunctionalization of alkenes using nitrogen-heteroatom bonds. **Q. Wang**

1:40 ORGN 276. Iodine-based reagents for alkene functionalizations. **T. Wirth**

2:20 ORGN 277. Recent advances in organocatalytic bromination reactions. **Y. Yeung**

3:00 ORGN 278. New halogenation strategies for the generation of unusual reactivities and selectivities. **T. Gulder**

3:40 ORGN 279. Asymmetric alkene and arene halofunctionalization reactions in meroterpenoid biosynthesis. **B.S. Moore**

4:20 ORGN 280. Catalytic, enantioselective *Syn* dichlorination. **S.E. Denmark**

Section D
Ernest N. Morial Convention Center
R04

Molecular Recognition & Self-Assembly

R.D. Broene, *Organizer*
J.L. Fantini, *Presiding*

1:20 ORGN 281. Peptides and peptidomimetics as anion receptors in aqueous solutions. **K. Jolliffe**

1:40 ORGN 282. Iodide speciation tuned by cyanostar self-assembly. **E.M. Fatila**, C. Benson, W. Zhao, M. Pink, J. Karty, A.H. Flood

2:00 ORGN 283. Molecular recognition in biomimetic membrane systems. **L. Perez**, R.J. Hooley

2:20 ORGN 284. Functionalized calixarenes: Synthesis, characterization and anion sensing applications. **N. Edwards**, I. Gearba, D.M. Schnable, F. Liu

2:40 ORGN 285. Pyrene-box capsules for adaptive encapsulation and structure determination of unstable or non-crystalline biogenic compounds. **M. Barboiu**

3:00 ORGN 286. Thermodynamics of PAMAM-carboxylate interactions using isothermal titration calorimetry. **N. White**, K.C. Glisson, M. Bonizzoni

3:20 ORGN 287. Thermal, crystallographic and spectroscopic studies on enantiomerically pure and racemic allylated mannoses showing self-assembling properties. **I. Mattsson**, M. Lahtinen, A. Peuronen, T. Saloranta-Simell, R. Leino

3:40 ORGN 288. Prescribed molecular recognition via shape mimicry. **K.A. Wheeler**, L.S. Cantrell, E.N. Pinter, I.C. Tinsley, B.L. Wagner

4:00 ORGN 289. Tetrasulfonatocalixarenes grafted at the methylene bridge position to multiwall carbon nanotubes for interaction with acetylcholine. **J.L. Fantini**, J.D. Sundberg, J. De La Torre, K. Sinniah

Section E
Ernest N. Morial Convention Center
R05

Materials, Devices & Switches

R.D. Broene, *Organizer*
M.R. Bryce, *Presiding*

1:20 ORGN 290. Improvement of charge mobilities for conjugated molecules and polymers through modifications of side alkyl chains. **D. Zhang**

1:40 ORGN 291. Autonomous materials: Triggered transience and targeted delivery. **A.M. Feinberg**, J.S. Moore

2:00 ORGN 292. NIR fluorescent indolizine-squaraine and indolizine-cyanine dyes. **J.N. Gayton**, L.E. McNamara, A. Huckaba, T. Rill, E.A. Sharpe, S. Autry, N. Hammer, J.H. Delcamp

2:20 ORGN 293. Stable water-soluble imaging probes based on upconverting nanoparticles functionalized with Janus-type dendrimers. **S. Plunkett**, M. El Khatib, I. Sencan, J. Collins, S. Sakadzic, S. Vinogradov

2:40 ORGN 294. New organic materials for thermally activated delayed fluorescence and light-emitting devices. **M.R. Bryce**

3:00 ORGN 295. Tailoring hole-transporting materials for perovskites solar cells. **A. Molina-Ontoria**, J. Urieta-Mora, I. García-Benitro, I. Zimmermann, J. Aragó, E. Ortí, M. Nazeeruddin, **N. Martin**

3:20 ORGN 296. Panchromatic photoresponsive dye-sensitized solar cell devices using thieno[3,4-b]thiophene-based photosensitizers. **P. Brogdon**, H. Cheema, J.H. Delcamp

3:40 ORGN 297. High voltage molecular engineered organic sensitizer-iron redox shuttle pair: 1.4 V DSC and 3.2 V SSM-DSC devices. **R.R. Rodrigues**, H. Cheema, J.H. Delcamp

4:00 ORGN 298. Building molecules with a programmable molecular robot. **S. Kassem**, A. Lee, D.A. Leigh, V. Marcos, L. Palmer, S. Pisano

Section F
Ernest N. Morial Convention Center
R03

Twenty Years of Organo- & Photoredox Catalysis

S.M. Silverman, *Organizer*
N. Goodwin, *Presiding*

1:00 ORGN 299. Oxidative functionalizations via visible light photoredox catalysis. **T.P. Yoon**

1:25 ORGN 300. Firmenich's quest towards sustainable synthetic ingredients. **M. Reiter**

1:50 ORGN 301. Discovery of a potent, selective and orally bioavailable RORc inverse agonist GNE-1032: Driving out PXR activation on an atypical norbornane scaffold. **J. Zbieg**, J. Crawford, O. Rene, S.M. Bronner, W. Lee

2:15 ORGN 302. Interdiction at a protein-protein interface: Structure-based design of the Mcl-1 inhibitor AMG 176. **S.P. Brown**

2:40 ORGN 303. Utilization of an active site mutant receptor for the identification of potent and selective atypical 5-HT2C receptor agonists. **J. Carpenter**, Y. Wang, G. Wu, J. Feng, X. Ye, C.L. Morales, M. Broekema, K.A. Rossi, K.J. Miller, B.J. Murphy, G. Wu, S.E. Malmstrom, A.V. Azzara, P.M. Sher, J.M. Fevig, A. Alt, R.L. Bertekap, M.J. Cullen, T. Harper, K. Foster, E. Luk, Q. Xiang, M.F. Grubb, J.A. Robl, D.A. Wacker

3:05 ORGN 304. Rethinking amidation chemistry: Development of a mild and direct lactamization protocol for the synthesis of pyridopyrazine-1,6-diones. **D.A. Rankic**

3:30 ORGN 305. Oxidative C-H functionalization. **S. Blakey**

3:55 ORGN 306. New transformations in synthesis via organic photoredox catalysis. **D.A. Nicewicz**

4:20 ORGN 307. Targeting the Kelch domain of KEAP1: A fragment-based discovery approach to identifying small molecule activators of Nrf2. **N.C. Goodwin**

4:40 ORGN 308. Recent advances in olefin amination. **R.R. Knowles**

Advances in Molecular Recognition of Double-Helical DNA & RNA
Sponsored by CARB, Cosponsored by MEDI and ORGN

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

‡*Cooperative Cosponsorship*

Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Homogeneous Catalysis for Applied Organic Synthesis
Sponsored by CATL, Cosponsored by INOR and ORGN‡

Homogeneous Catalysis for Applied Organic Synthesis
Sponsored by CATL, Cosponsored by INOR and ORGN‡

At the Frontier of Stereoselective Alkene Halofunctionalization
Cosponsored by ORGN

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
S.M. Silverman, *Organizer*

8:00–10:00

112, 121, 123, 125-129, 131, 133-134, 136-137, 144, 152, 158, 160, 162, 168, 172, 176-177, 183, 193, 204. See previous listings.

409, 418-419, 424, 429, 434, 436, 442, 446-447, 449, 454, 458-459, 461-462, 467, 470-471, 473, 484, 490, 494, 498, 507-508, 510, 512, 515, 621, 628, 632, 634, 641, 647, 661, 687, 693, 699-701, 703, 705, 715, 725, 732, 741. See subsequent listings.

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

Josef Michl ACS Award in Photochemistry: Symposium in honor of Jack Saltiel

M.K. Boyd, E.C. McLaughlin, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 309. Alkyne photochemistry for double DNA-cleavage and for the uncaging of aldehydes. **I. Alabugin**

8:40 ORGN 310. Moving charge through duplex DNA: Injection, separation, transport and trapping. **F.D. Lewis**, R. Young, M.R. Wasielewski

9:15 ORGN 311. Chameleon materials: Imidazole imidazolium substituted polythiophenes. Photophysical properties, photochemistry and biological activity. **D.G. Whitten**, J. Zhang, D. Brown

9:50 ORGN 312. Medium matters: Merging photochemistry with supramolecular-, nano- and green chemistry. **V. Ramamurthy**

10:25 ORGN 313. Interrogating the photochemistry of caged functional groups: Hidden mechanistic variations. **R.S. Givens**

11:00 ORGN 314. Award Address (Josef Michl ACS Award in Photochemistry Sponsored by the Josef Michl Award Endowment). Trapping twisted intermediates in cis-trans photoisomerization. **J. Saltiel**, S. Gupta

Section B
Ernest N. Morial Convention Center
R02

Complex Synthetic Chemistry with Simple Starting Materials

U.K. Tambar, *Organizer, Presiding*

8:00 ORGN 315. Redox catalysis strategies for complex molecules. **C. Stephenson**

8:30 ORGN 316. Constructing C–N and C–O bonds with spatial control. **J. Read De Alaniz**

9:00 ORGN 317. Construction of highly strained molecular hoops, belts, and cylinders. **R. Jasti**

9:30 ORGN 318. Natural products in the atmosphere. **R.J. Thomson**

10:00 ORGN 319. New methods for carbonyl-olefin metathesis. **C. Schindler**

10:30 ORGN 320. Wielding the power of social media for scientific scholarship and advocacy. **T.I. Asino**

Section C
Ernest N. Morial Convention Center
R01

Heterocycles & Aromatics

R.D. Broene, *Organizer*
K. Miller, *Presiding*

8:20 ORGN 321. Synthesis of quinoline-5,8-dione containing isoxazoles and isoxazolines. **R.E. Sammelson**, R. Ravanfar, M.J. Campbell, S. Stump, H.D. Beall

8:40 ORGN 322. Oxindole as a versatile scaffold: A promising heterocycle for the development of potent anti-cancer active agents. **A. Barakat**, H.M. Ghawas, M.S. Islam, A. Al-Majid, F. El-Senduny, F. Badria

9:00 ORGN 323. Application of the transition-metal free cross coupling of sulfonylhydrazones and boronic acids to the total synthesis of avrainvilleol. **K. Miller**

9:20 ORGN 324. Discovery of copper-activated heterocyclic compounds as new therapeutic strategy for combating gram-positive bacteria. **M. Zhang**, A. Delpe Acharige, M. Kalubowilage, F. Wolschendorf, S.H. Bossmann

9:40 ORGN 325. Dearomatization strategies in the synthesis of complex heterocyclic natural products. **J. George**

10:00 ORGN 326. Synthesis of tri-substituted quinolines as drug candidates for HIV-1 integrase inhibition. **A. Hart**, N.G. Jentsch, J. Hume, J.A. Pigza, J. Kessl, J. Sun, M.G. Donahue

10:20 ORGN 327. Modular diversification of heteroaromatic complexant scaffolds for separations using metal-mediated coupling strategies. **J.D. Carrick**

10:40 ORGN 328. Catalytic use of a calcium-based Lewis acid for the synthesis of heterocyclic compounds. **V. Gandon**

Section D
Ernest N. Morial Convention Center
R04

Molecular Recognition & Self-Assembly

R.D. Broene, *Organizer*
B.W. Purse, *Presiding*

8:40 ORGN 329. Reverse Hofmeister effects in synthetic hosts. **J.H. Jordan**, C.L. Gibb, W. Yao, A. Wishard, B.C. Gibb

9:00 ORGN 330. Electrochemiluminescent chemodosimetric probes for selective detection of biological and environmental targets. H. Kim, S. Kim, K. Kim, **J.I. Hong**

9:20 ORGN 331. Molecular recognition and sensing of nucleotides with a dinuclear copper(II) complex in water. **A. Hossain**, M. Rhaman, D.R. Powell

9:40 ORGN 332. Fluorescent-based biosensors for detection of human serum albumin protein. **R. Choudhury**

10:00 ORGN 333. Minimal oligonucleotide length required for the assembly of the cowpea chlorotic mottle virus. S. Maassen, M. de Ruiter, **J.J. Cornelissen**

10:20 ORGN 334. Kinetics of formation of the host-guest complex of zwitterionic viologen with cucurbit[7]uril. **Y. Zheng**, A.E. Kaifer

10:40 ORGN 335. MAMBA[n]arenes: Functionally diverse amide-bridged container molecules. **J.W. Meisel**, A.D. Hamilton

11:00 ORGN 336. Withdrawn

Section E

Ernest N. Morial Convention Center
R05

New Reactions & Methodology

R.D. Broene, *Organizer*
C. Brindle, *Presiding*

8:20 ORGN 337. New insights into the production of platform chemicals from biomass using deep eutectic solvents. **T. Istasse**, M. Kammoun, A. Richel

8:40 ORGN 338. Regioselective, solvent- and metal-free approach to access 3-Se/S-chromones from the cyclization of enaminones employing I_2/DMSO as an eco-friendly catalytic oxidation system. **J. Khan**, **S. Saba**, A.R. Schneider, T.L. Luciano, M.S. Franco, **A.L. Braga**

9:00 ORGN 339. Recent advances in halogen bond catalysis. **P.H. Toy**

9:20 ORGN 340. Synthesis and deployment of enantiomerically pure 3-substituted-piperazine-2-acetic acid esters as templates for FBLD. **S. Guduru**, C. Santini, D.W. Young

9:40 ORGN 341. Synthesis of novel bicyclic amines and their application for drug discovery. **P. Mykhailiuk**

10:00 ORGN 342. Stereoselective synthesis of tri- and tetrasubstituted β,β-difluoro-β-oxo alkenes by free-radical reaction of iododifluoromethyl ketones. J. Wu, J. Liang, D. Wang, **F.H. Wu**

10:20 ORGN 343. Dynamic kinetic resolution of tetrasubstituted olefins. **J. Majhi**, B.W. Turnbull, H. Ryu, J. Park, M. Baik, P. Evans

10:40 ORGN 344. Difluorocyclopropanation of functionalized alkenes using CF_3SiMe_3–NaI system. **S. Ryabukhin**, P. Nosik, O. Grygorenko, D. Volochnyuk

11:00 ORGN 345. Purification of mixtures using bisulfite: Facile separation of aldehydes and ketones through reversible bisulfite adduct formation. **C. Brindle**

Section F
Ernest N. Morial Convention Center
R03

Photoredox Chemistry

R.D. Broene, *Organizer*
T. Knauber, *Presiding*

8:00 ORGN 346. Copper-based complexes for photocatalysis. **S.K. Collins**

8:20 ORGN 347. Development of a Ru/Ni dual catalytic desulfinative photoredox Csp^2-Csp^3 cross-coupling. **T. Knauber**

8:40 ORGN 348. Visible-light promoted C-S, C-N, and C-C bond-forming reactions: Applications and mechanistic studies. **M.S. Oderinde**, J.W. Johannes, M. Frenette, P. Nuhant, O. Fadeyi, J. Genovino

9:00 ORGN 349. Light harvesting for rapid and selective reactions: Click chemistry with strain-loadable alkenes. **K. Singh**, C. Fennell, E. Coutsias, R. Latifi, S. Hartson, J.D. Weaver

9:20 ORGN 350. Withdrawn

9:40 ORGN 351. Cross-electrophile coupling of activated alkyl halides and aryl halides via metallaphotoredox catalysis. **T.Q. Chen**, D.W. MacMillan

10:00 ORGN 352. Activation of aryl halides towards cross-coupling technology via metallaphotoredox catalysis. **C. Le**, T.Q. Chen, T. Liang, D.W. MacMillan

10:20 ORGN 353. Photocatalytic generation of 2-azolyl radicals: Intermediates for the azolylation of arenes and heteroarenes via C-H functionalization. **A. Arora**, J.D. Weaver

10:40 ORGN 354. Metallaphotoredox catalysts for late stage functionalization. **J. Kautzky**, T. Wang, R.W. Evans, D.W. MacMillan

11:00 ORGN 355. C–H arylation via the merger of photoredox, hydrogen atom transfer and nickel catalysis. **M.H. Shaw**, V.W. Shurtleff, J.A. Terrett, J.D. Cuthbertson, D.W. MacMillan

‡*Cooperative Cosponsorship*

11:20 ORGN 356. New strategies for C—C bond formation enabled by metallaphotoredox catalysis. **I. Perry**, T. Brewer, D.W. MacMillan

11:40 ORGN 357. Oxidative [1,2]-Brook rearrangements exploiting single-electron transfer: Photoredox-catalyzed alkylations and arylations. **Y. Deng**, Q. Liu, A.B. Smith

Recent Advances in Catalytic Carbohydrate Reaction Development
Sponsored by CARB, Cosponsored by ORGN

ACS Award for Encouraging Women into Careers in the Chemical Sciences

Symposium in Honor of Rebecca Ruck

Sponsored by WCC, Cosponsored by ORGN, PROF and YCC‡

Homogeneous Catalysis for Applied Organic Synthesis
Sponsored by CATL, Cosponsored by INOR and ORGN‡

Homogeneous Catalysis for Applied Organic Synthesis
Sponsored by CATL, Cosponsored by INOR and ORGN‡

Advances in Molecular Recognition of Double-Helical DNA & RNA
Sponsored by CARB, Cosponsored by MEDI and ORGN

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in honor of Seth B. Herzon

Cosponsored by MEDI
S.M. Sieburth, *Organizer, Presiding*

1:00 ORGN 358. Selective catalytic reactions in complex molecular environments inspired by natural products. **S.J. Miller**

1:50 ORGN 359. Bringing the full power of chemical synthesis to bear on the discovery of new antibiotics. **A.G. Myers**

2:40 ORGN 360. Translational chemistry. **P.S. Baran**

3:30 Introduction of Awardee.

3:35 ORGN 361. Award Address
(Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator Sponsored by the Pfizer Endowment Fund). Synthesis and study of isolated and predicted natural products. **S. Herzon**

Section B
Ernest N. Morial Convention Center
R02

Discovery of Small Molecules Targeting RNA
Cosponsored by CARB and MEDI
S.C. Zimmerman, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 362. Aminoglycoside binding to ribosomal RNAs: New compounds and new targets. **C.S. Chow**

1:30 ORGN 363. High-throughput platform assay technology for the discovery of pre-microRNA-selective small molecule probes. **A.L. Garner**

1:55 ORGN 364. Discovery and application of cheminformatics-derived principles for small molecule:RNA targeting. B. Morgan, J.E. Forte, A. Donlic, N.N. Patwardhan, **A.E. Hargrove**

2:20 ORGN 365. Targeting HIV-1 Rev response element with branched peptides. **W.L. Santos**

2:45 Intermission.

3:15 ORGN 366. Targeting structurally and functionally diverse RNAs with druglike small molecules. **J.S. Schneekloth**

3:40 ORGN 367. Isomorphic and isofunctional fluorescent nucleosides and nucleotides for studying RNA-centric processes. **Y. Tor**

4:05 ORGN 368. Pervasive role for structure in ncRNA and mRNA function. **K.M. Weeks**

4:30 ORGN 369. To splice or not to splice: Can small molecules answer the question? **M.G. Woll**, G.M. Karp, N.A. Naryshkin, C.R. Trotta, M. Weetall, A. Bhattacharyya, A. Dakka, K.A. Effenberger

4:55 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
R01

Heterocycles & Aromatics

R.D. Broene, *Organizer*
M.R. Nahm Garrett, *Presiding*

1:20 ORGN 370. Competitive photoinduced energy and electron transfer in porphyrin- fullerene triad. **Y. Hu**, M. Thomas, R. Jinadasa, F. D'Souza, H. Wang

1:40 ORGN 371. Synthesis of tetracenes: A possible means of achieving renewable energy. **M.R. Nahm Garrett**, S. Woodward

2:00 ORGN 372. Constructing extended pi-conjugated systems using dynamic bonds. **L. Fang**

2:20 ORGN 373. Ladder-type π-conjugated molecules and macromolecules featuring boron-nitrogen coordinate bonds. **C. Zhu**, L. Fang

2:40 ORGN 374. Aurones: Opening doors to a whole new yellow. **J. Schmitt**, S. Handy

3:00 ORGN 375. Tridecacyclene: Synthesis, properties, and aromaticity of a congested cyclooctatetraene. **A. Whalley**

3:20 ORGN 376. Synthetic strategies relative to rearrangments featured in the palladium catalyzed arene-triflate ring closing reaction. **G.S. Pour**, R. Ly, K.D. Trieu, D.C. Fairchild, A. Burnstine-Townely, D.A. Vazquez-Molina, A.D. Campiglia, J.K. Harper, F.J. Uribe-Romo

3:40 ORGN 377. New red-photocleavable dyes with high aqueous efficiency. **X. Wang**, J.A. Kalow

Section D
Ernest N. Morial Convention Center
R04

Molecular Recognition & Self-Assembly

R.D. Broene, *Organizer*
M. Best, *Presiding*

1:20 ORGN 378. pH-switched self-assembly of a self-complementary supramolecular motif in polar solvent. **X. Duan**, J.W. Canary

1:40 ORGN 379. Stimuli-responsive anion-based supramolecular polymers. **W. Zhao**, B. Qiao, A.H. Flood

2:00 ORGN 380. Dynamic communication through reorganizable hydrogen bond networks. **D. Tilly**, D.T. Morris, J. Ward, J. Clayden

2:20 ORGN 381. G-quadruplex formation from H8 modified guanosine derivatives: From structure to function. **Y. He**, X. Shi

2:40 ORGN 382. *In situ* synthesis of dynamic phospholipid membranes. **A. Seoane Fernandez**, R.J. Brea, A. Fuertes, N.K. Devaraj

3:00 ORGN 383. Continual reproduction of self-assembling peptide nanomaterials. **R.J. Brea Fernández**, N.K. Devaraj

3:20 ORGN 384. Strategies for triggering liposome membrane fusion and content release. **M. Best**, J. Lou, A.M. Bayer, S. Whitehead, A.J. Carr, X. Zhang, S. Alam, S.I. Mattern-Schain, A.J. Watson

3:40 ORGN 385. Meta-stable homoleptic complexes as a supramolecular springboard for the formation of heterocomplexes. **P.M. Bogie**, L.R. Holloway, C. Ngai, Y. Lyon, R. Julian, R.J. Hooley

Section E
Ernest N. Morial Convention Center
R05

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

R.D. Broene, *Organizer*
P. Wiget, *Presiding*

1:00 ORGN 386. Gas-phase reactivity study of aromatic biradicals containing both β- and π-type radical sites. **X. Ma**, Z. Yu, J.J. Nash, H.I. Kenttamaa

1:20 ORGN 387. Halocarbenes may deplete atmospheric ozone. **A. Mamantov**

1:40 ORGN 388. Experimental and computational synergy for sustainable chemical recycling. **G.O. Jones**

2:00 ORGN 389. Mechanisms of molecular-iodine-catalyzed reactions. **M. Breugst**, D. von der Heiden, E. Detmar

2:20 ORGN 390. Long-range donor-acceptor effects in heterocyclic medium-sized rings: Structural analysis, perlin effects, and anchimeric assistance. **P. Wiget**

2:40 ORGN 391. Anilinium salts in methylation reactions: An experimental and computational study. **M. Reid**

3:00 ORGN 392. Theoretical studies of mechanisms and selectivities of metal-catalyzed fluorination reactions. **F. Himo**

3:20 ORGN 393. Helical conformations in per- and polyfluorinated substances: Origins, energies, and stability. D.J. Van Hoomissen, M. Pagenkopf, **S. Vyas**

3:40 ORGN 394. Synthesis and experimental evaluation of cationic gold (I) carbene complexes relevant to gold (I) catalysis. **R. Carden**, N. Lam, N. Stevenson, R. Widenhoefer

4:00 ORGN 395. Reaction mechanism as a novel approach to tune the site selectivity of transition metal catalyzed intramolecular nitrene transfer: An example using silver complexes. **T. Yang**, J.F. Berry

4:20 ORGN 396. Gas phase benzyl, tropylium cations rearrangement reinvestigated using accurate mass quadrupole time of flight gas chromatography mass spectrometry (GCQTOF). T. Nguyen, M. Aparicio, **M.A. Saleh**

4:40 ORGN 397. Unveiling the photochemistry of diamidocarbenes. **T.W. Hudnall**, T.A. Perera

Section F
Ernest N. Morial Convention Center
R03

Photoredox Chemistry

R.D. Broene, *Organizer*
J.D. Weaver, *Presiding*

1:00 ORGN 398. Photoredox-mediated ring-opening metathesis polymerization: Methods, scope, and scalability. **L.M. Pascual**, A.J. Boydston, P. Lu, V. Kensy, D.C. Lee, N. Alrashdi

1:20 ORGN 399. Withdrawn

1:40 ORGN 400. Direct aryl C–H amination using primary amines via organic photoredox catalysis. **A. Levens**, K. Margrey, D.A. Nicewicz

2:00 ORGN 401. Cation radical accelerated nucleophilic aromatic substitution via organic photoredox catalysis. **N. Tay**, D.A. Nicewicz

2:20 ORGN 402. Structure-property relationships for tailoring phenoxazines as reducing photoredox catalysts. **B. McCarthy**

2:40 ORGN 403. Development of light absorbing organic molecules for photoredox catalysis. **M.V. Bobo**, A.K. Vannucci

3:00 ORGN 404. Iterative photocatalytic C-H functionalization; rapid and programmable access to oligioarenes. **J.D. Weaver**

‡*Cooperative Cosponsorship*

3:20 ORGN 405. Spin-center shift-enabled direct enantioselective alpha-benzylation of aldehydes with alcohols. **E.D. Nacsa**, D.W. MacMillan

3:40 ORGN 406. Decarboxylative alkylation for site-selective bioconjugation of native proteins via oxidation potentials. **S. Bloom**

4:00 ORGN 407. Strain induced couplings mediated by visible light. **K. Singh**, W. Trinh, J.D. Weaver

4:20 ORGN 408. Mechanistic analysis of photocatalytic cross-coupling reactions. **N. Till**, M. Shaw, E. Corcoran

Recent Advances in Catalytic Carbohydrate Reaction Development
Sponsored by CARB, Cosponsored by ORGN

Homogeneous Catalysis for Applied Organic Synthesis
Sponsored by CATL, Cosponsored by INOR and ORGN‡

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

Biologically Related Molecules & Processes

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 409. Spirooxindole analogues as a new class of anti-cancer and anti-inflammatory active agents. **G.L. Elarag**, E. El Ashry, M. Said, E. El Tamany, S. Yousuf, M. Choudhary, A. Barakat

ORGN 410. Synthesis of a novel small molecule inhibitor of D14-type strigolactone receptors. **S.F. Kim**, R. Takise, M. Yoshimura, S. Hagihara, K. Itami

ORGN 411. Development of DNA-compatible Suzuki-Miyaura reaction in aqueous media. **J. Li**, H. Huang

ORGN 412. Drug design, synthesis, and characterization of photo-isomerizable drugs with novel application in pharmaceutical and biochemical research. **M. Kazmierczak**, C. Streu, Z. Dill

ORGN 413. Understanding the function of active site residues and an ordered loop of an *Oryza sativa* tyrosine aminomutase towards parsing its mutase and lyase activities. **G.K. Attanayake**, T. Walter, K.D. Walker

ORGN 414. Progress toward the synthesis of an azo-derivative of a hedgehog signaling pathway inhibitor. **Z. Dill**, C. Streu

ORGN 415. Toward a total synthesis of a spin labeled phosphoramidon derivative and TEMPO conjugation of ilomastat for the creation of EPR chemical probes. **M. Nazario**, D.A. Hunt, D.J. Hirsh

ORGN 416. New compound, *N-(n-anisyl)ethyl-N-Methylcinnamamide* extracted from *Zanthoxylum clava-herculis* tree bark. **Y.H. Kim**, K. Moon, Z. Riley, M. Richardson

ORGN 417. Mitochondrial-targeted organic photoCORM. **T. Soboleva**, H.J. Esquer, A. Benninghoff, L.M. Berreau

ORGN 418. Synthesis of dimeric naphthalene derivatives for recognition of DNA. **B. Chavez**, **R. Shaktah**, T.G. Minehan

ORGN 419. Preventing outer membrane formation in Gram-negative bacteria: Design and synthesis of inhibitors of LpxC. **A.O. Pajarillo**, R.J. Roldan, C.P. Embry, S.N. Malkowski, G.G. Lamanilao, M.L. Cafiero, L.W. Peterson

ORGN 420. Synthesis of novel catecholic derivatives and evaluation as COMT inhibitors. **G. Kennedy**, A.K. Hatstat, C. Cochrane, M.L. Cafiero, L.W. Peterson

ORGN 421. Reaction based chemiluminescent probe for nitroreductase and hypoxia *in vivo*. J. Cao, **L.S. Ryan**, A.R. Lippert

ORGN 422. Synthesis of mannose building blocks for preparation of O-mannosylated glycans. **K. Zhao**, J.L. Koviach-Cote

ORGN 423. Design and synthesis of non-nucleoside as potential inhibitors of LpxC. **C. Embry**, R. Roldan, A.O. Pajarillo, M.L. Cafiero, L.W. Peterson

ORGN 424. Synthesis and properties of porphyrin-carbohydrate conjugates for use in photodynamic therapy. **A.V. Delos Reyes**, D.R. Mootoo, P. Gonzalez, N. Bhupathiraju, C.M. Drain

ORGN 425. Isolation and characterization of alkaloids from *Lupinus albifrons* and *Tecoma capensis*. **C.A. Sanchez**, P.M. Joyner

ORGN 426. Synthesis and characterization of novel 3,5-diaryl-Δ^1-pyrroline-5-carbonitriles as potential breast cancer cells inhibitors. V. Mihaylova, D. Tasheva, I. Ivanov, **N.N. Mateeva**

ORGN 427. Development of a water soluble antioxidant dendrimer from naturally available vanillin. **H. Brinkman**, C.Y. Lee, A. Ausmus, C. Anamoah, R. O'Connell

ORGN 428. Novel quinolinedione for reductive generation of a visible light-triggered CO-releasing molecule in biological systems. **M. Popova**, T. Soboleva, L.M. Berreau

ORGN 429. Combating drug resistant cancer: Inhibiting glutathione s-transferase via ethacrynic acid derivatives. **T.A. Cooley**, I. Janser, T.L. Friebe

ORGN 430. Utilizing protein prenylation to modify EpCAM targeting DARPins with an azide-containing isoprenoid analogue. **S.A. Auger**, Y. Zhang, J. Schaefer, A. Plückthun, M.D. Distefano

ORGN 431. Development of 4-hydroxy-N-propyl-1,8-napthalimide acyloxymethyl ethers for characterization of esterase activity. **E. Larsen**, R. Johnson

ORGN 432. Synthesis and computational evaluation of vorinostat boron derivatives as potential histone deacetylase inhibitors. **B. Rich**, **E. Goldman**, C. Martin, S. Stoddard, K.A. Brien

ORGN 433. Synthesis of the Xyl-GlcA disaccharide repeat of the m3 O-mannosylated glycan. **C. Merton**, **J.L. Koviach-Cote**

ORGN 434. Penetrating Gram-negative bacteria – unlocking spatial effects upon transport. **P.K. Desman**, T. Nguyen, V. Hoang, Y. Zhang, R.J. Rafferty

ORGN 435. Investigations into blood-brain barrier transport: Effects of physicochemical properties and small molecule chaperone synthesis. **K. Ferguson**, W.W. Hulangamuwa, A. Fatino, R.J. Rafferty

ORGN 436. Bioactive molecule discovery via intermediates of total synthesis. **O. Haney**, V. Hoang, Y. Zhang, P. Desman, R.J. Rafferty

ORGN 437. Marketing the heparinic building blocks for expanding the access to the synthetic heparinoids. **S. Nadji**

ORGN 438. Synthesis and biological activity of novel 1,3-oxazole sulfonamides. **E. Almanasrah**, K. Barnes

ORGN 439. Synthesis of more metabolically stable analogs of the bromodomain inhibitor (+)-JQ1 using chemical metabolic soft spot mapping. **K.B. Guzman**, J.C. Williams, S.L. Holmes, P. Jain, F. Li, C. Santini, D.W. Young

ORGN 440. Separation of biofuels from ionic liquids via reversible solubility. **R. Wolsleger**, R.E. Del Sesto

ORGN 441. Stabilizing the collagen triple helix via covalent and non-covalent approaches. **J.M. Keever**, P.D. Banzon, W.E. Allen

ORGN 442. Development of fluorogenic probes for sugar transport analysis. **A. Ferrier**, V.V. Begoyan, M. Tanasova

ORGN 443. Fluorescent derivatives of prostaglandins: Tools for studying anti-cancer activity. **J.L. Stanley**, R. Van Dross, W.E. Allen

ORGN 444. Membrane localization of pyrene-trehalose conjugates (PYRETs). **A.M. Hagwood**, A.M. Kennedy, W.E. Allen

ORGN 445. Does substance P sequester anions in membranes? Implications for cellular [Cl^-]. **M. Muhammad**, A.L. Sargent, W.E. Allen

ORGN 446. Brominated nucleosides for aromatic substitution: Synthesis and *in vitro* studies. **C.S. Jacobsen**, C.W. McLaughlin

ORGN 447. Nitrodibenzofuran photoactivatable protecting group with longer wavelength absorption for orthogonal activation of biological thiols. **A.D. Fenton**, **S. Fang**, **M. Hammers**, M.D. Distefano

ORGN 448. Unveiling the conformational preferences of fructose transporters. **V.V. Begoyan**, L.J. Weselinski, M. Tanasova

ORGN 449. Structural optimization of atropisomeric pyrrolopyrimidine RET kinase inhibitors. **S. Toenjes**, **V. Garcia**, J. Gustafson

ORGN 450. Spiro-peroxo-isoxazolines: Halo-peroxidation mediated three step syntheses of potential novel anti-malarial and anti-cancer peroxide analogues. **P. Das**, A. Hamme

ORGN 451. Rational design of stapled peptides to target the CHP1-NHE1 protein-protein interaction. **R. Noorbehesht**, C.J. Nalbandian, J. Gustafson

ORGN 452. Development of a chemiluminescent probe for nitroxyl. **W. An**

ORGN 453. Formation and testing of ketoacid derivatives as possible treatment for improper leucine metabolism. **V. Cinnater**, A. Ramanathan, C.J. Stephenson

Section A
Ernest N. Morial Convention Center
Hall D

Chemistry of Fullerenes, Carbon Nanotubes & Graphene

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 454. Ni-Pd nanoparticle @ Graphene-nanotube hybrids as robust catalysts in cross-coupling reactions. **Y. Yang**, M. Burkholder, S. Gilliland, C.E. Castano, F. Gupton

ORGN 455. Effect of graphene support on the activity of first-row transition metal clusters for cross-coupling reactions. **Y. Yang**, A.C. Reber, S. Gilliland, C.E. Castano, S.N. Khanna, F. Gupton

ORGN 456. Improved syntheses of cyclopenta[l,m,n]phenanthrenes: Precursors for large scale preparation of corannulene. D.J. Marquardt, **P. LaPlant**

Section A
Ernest N. Morial Convention Center
Hall D

Flow Chemistry & Continuous Processes

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 457. Efficient synthesis of antimalarial drug hydroxychloroquine in continuous flow. **H.R. Mangunuru**

ORGN 458. NSERC CREATE program in continuous flow science. **V. Kairouz**, S.K. Collins, A.B. Charette

ORGN 459. Synthesis of primary amine HX salts from halides and ammonium hydroxide in continuous flow chemistry. **A. Bouchard**, C. Audubert, H. Lebel

ORGN 460. Iron-catalyzed amination of thioethers and sulfoxides in continuous flow. **C. Lai**, H. Lebel

ORGN 461. Optimization of hylene MP synthesis for production via microfluidics. **S.M. Torres**, T. Robison, Z.S. Peacock

Section A
Ernest N. Morial Convention Center
Hall D

Materials, Devices & Switches

S.M. Silverman, *Organizer*

‡*Cooperative Cosponsorship*

5:30–7:30

ORGN 462. Advances in hypersorbent materials for detection and protection applications. **C.A. Roberts**, R.A. McGill, M.R. Papantonakis, T. Grissom, A. Kusterbeck

ORGN 463. Controlling alignment of donor-acceptor columnar liquid crystals using laser irradiation. **M. Van Winkle**, B. Kaehr, J.J. Reczek

ORGN 464. Propeller-shaped Pi-expanded coumarins as aryl-aryl dihedral angle switches. **S.M. Meyer**, H.A. Hintz, N. Sortedahl, B.J. Dahl

ORGN 465. Oligoethylene glycol solubilized crankshaft lactone molecular switches. **E.M. Charlesworth-Seiler**, J.J. Dressler, Y. Torres, B.J. Dahl

ORGN 466. Synthesis and characterization of electron-donating and electron-accepting perylene diimide derivatives for use in organic photovoltaic devices. **R. de Dios**, S. Archuleta, L. Mier

ORGN 467. Synthesis and characterization of charge transfer complexes of sulfur-rich aromatic compounds. **Q. Qin**, H. Gould

ORGN 468. New unsymmetrical flex-boxes: Flexible viologens cyclophanes. J. Richard, J. Wytko, **C. Boudon**, S. Choua, R. Laurent, **J. Weiss**

ORGN 469. Evidence of iodine binding with thiophene based dyes in DSCs. **A. Baumann**, H. Cheema, L.E. McNamara, S. Nguyen, D.L. Watkins, N. Hammer, J.H. Delcamp

ORGN 470. Synthesis of novel photochromic azobenzene derivatives. **K. Mohamed**

ORGN 471. Molecular switching of tris(azobenzene)amine. **K.S. Strickland**, C.J. Saint-Louis, S.C. Blackstock

ORGN 472. Synthesis and characterization of high-capacity swellable organically-modified silica. **P.A. Bonvallet**, T. Branscum, Z. Thornburg

ORGN 473. Structural effects on the rotational barrier atropisomeric rhodamine derivative. D. Rich, **M. Bollinger**, N.Y. Aleman, **T. Gaston**, L.V. Odom, V. Cinnater, C.J. Stephenson

ORGN 474. Radical substituted phenylene diamines and oligoanilines: Models for organic spintronic systems. **W. Guan**, **I. Kwong**, **Y. Chen**, **Y. Mo**, D.J. Brook

ORGN 475. Synthesis and characterization of imide heteroaromatic polycyclic chromophores. **A. Taylor**, **H.D. Castonguay**, A. Schrock, M.T. Huggins, A. Bolin, B. Brown, C. Saint-Louis

ORGN 476. Effect of donor strength and bulk on thieno [3,4-b]pyrazine-based panchromatic dyes in dye-sensitized solar cells. **N. Liyanage**, H. Cheema, A. Baumann, A. Zylstra, J.H. Delcamp

ORGN 477. Novel ullazine-based organic dyes for dye-sensitized solar cells. **Y. Zhang**, H. Cheema, J.H. Delcamp

Section A
Ernest N. Morial Convention Center
Hall D

Molecular Recognition & Self-Assembly

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 478. Naked-eye detection of sulfate by a tripodal-based thiourea receptor. **A. Hossain**, M. Emami Khansari, M.H. Hasan, R. Tandon

ORGN 479. Selective post-assembly oxidations of self-assembled complexes containing reactive alkyl chlorides or activated CH groups. **L.R. Holloway**, R.J. Hooley

ORGN 480. Withdrawn

ORGN 481. Preparation of a water soluble metal-organic molecular cube using azo coupling of polyethylene glycol chains. **M.M. Mitchler**, J.D. Thoburn

ORGN 482. Uncharacteristic quasiracemic assemblies derived from tartramide/malamide molecular frameworks. **L.S. Cantrell**, E.N. Pinter, G. Day, K.A. Wheeler

ORGN 483. Sequence-specific folding of cucurbit[8]uril-bound β-hairpin peptides. **H. Clements**, M. Matsumoto

ORGN 484. ATP driven release of an enzyme inhibitor from cucurbit[7]uril using a DNA chimera based signal transducer. **X. Zhou**, P. Pathak, L.D. Isaacs, J. Jayawickramarajah

ORGN 485. Synthesis of an enlarged M_8L_6 metallocube. **E.M. Tiernan**, J.D. Thoburn

ORGN 486. Synthesis of pentahelicene and tetracyanoazulene: Two new aromatic guests for supramolecular metallocage encapsulation. **N.B. Herrington**, J.D. Thoburn

ORGN 487. Synthesis toward a molecular container based on *p-tert*-butylcalix[4]arene with gating features. **D. Balasooriya**, Y. Li, Z. Yan

ORGN 488. Nanohoop ligands: New cylindrical molecular building blocks for metal-organic self-assembly. **J. Van Raden**, S. Louie, R. Jasti

ORGN 489. Synthesis and physical analysis of an interdigitated capsule. **O.M. Munoz**, **J. Saldana**, L.M. Tunstad

ORGN 490. Self-assembly of pentameric macrocycles through alkene metathesis of bis(4-vinylbenzene)methyl derivatives. **J. Romo**, D.D. Cao

ORGN 491. Noncovalent interactions between PAMAM dendrimer analogues and carboxylates. **A.M. Iszler**, N. White, M. Bonizzoni

ORGN 492. Tuning the properties of pyrimidine for halogen bond driven supramolecular assembly. **D. Ngo**, S. Nguyen, T.L. Ellington, A.L. Rheingold, G.S. Tschumper, D.L. Watkins

ORGN 493. Controlling the solid-state self-assembly of [n]cycloparaphenylenes through weak organofluorine interactions. **E. Leonhardt**, J. Van Raden, R. Jasti

Section A
Ernest N. Morial Convention Center
Hall D

Nanomaterials

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 494. C-O bond activation catalyzed by UiO-66 supported Pd-Ni bimetallic nanoparticles. **J. Zhang**, C. Cai

ORGN 495. High performance polymeric nanocomposites from phthalonitrile resin and silane surface modified Ti_3AlC_2 MAX phase nanoparticles. **M. Derradji**, W. Liu

ORGN 496. Electrical conductivity and spectroscopic characterization of modified carbon nanotubes. **J.M. Hahn**

ORGN 497. Palladium nanoparticle-halloysite nanocomposites. Synthesis, characterization and catalytic activity. **J. Hamdi**, A. Blanco, J.B. Wiley, M.L. Trudell

Section A
Ernest N. Morial Convention Center
Hall D

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

S.M. Silverman, *Organizer*

5:30–7:30

ORGN 498. Untangling the mechanism of chlorocarbene additions to dibenzocyclooctyne. **A. Nadeem**, **A. Urquilla**, **Y. Saperstein**, D.C. Merrer

ORGN 499. Confronting the complexity of nonlinear systems. Acid-dependency of the Fe-catalyzed Belousov-Zhabotinsky oscillating chemical reaction. **E. Zars**, M. Delarosa, C. Chicone, R. Glaser

ORGN 500. Inhibition of CYP11B1 11β-hydroxylation by *Sutherlandia frutescens:* Theoretical studies of the active site and of steroid oxidation. **C. Hawkins**, **K. Chetney**, R. Glaser, W. Folk

ORGN 501. 2,3,5,6-Tetramethyl-1,4-di(N-nitrosoacetamido)benzene: An unusually stable N-aromatic-N-nitrosamide. **M.B. Houck**, D.R. Powell, D.T. Glatzhofer

ORGN 502. Computational study of regioselective Diels-Alder and diastereoselective Claisen rearrangement transition states. **K. Kron**, D.A. Vosburg, G.W. Daub, R.J. Cave

ORGN 503. Computational studies on regio- and diastereoselection in ketal Claisen rearrangements. G. Phun, **G.W. Daub**, R.J. Cave

ORGN 504. Stabilizing effects in the photochlorination and photobromination of haloalkanes. **A. LaPorte**, N. Mielke, D.J. Rausch, J.A. Bjorklund

ORGN 505. Taming of carbon-free energetic complexes consisting of all-nitrogen pentazole anion, metal cation, and H_2O. **Y. Xu**, M. Lu

ORGN 506. Computational study of 4-isoxazolines, 2-acylaziridines, and 4-oxazolines rearrangements. **P.A. Sibbald**

ORGN 507. Synthesis and reactions of pentacyclo[4.3.0.$0^{2,4}$.$0^{3,8}$.$0^{5,7}$]non-4-ene. **E. Brutschea**, **L. Bui**, **A. Tallon**, M.A. Forman

ORGN 508. Synthesis of iodinated precursors to pentacyclo[4.3.0.$0^{2,4}$.$0^{3,8}$.$0^{5,7}$]non-4-ene. **I. Armento**, **F. Baccari**, M.A. Forman

ORGN 509. Synthesis of selectively deuterated tetra(benzyloxy)benzenes for the purpose of elucidating ESI/CID fragmentation pathways. **J.E. McGettigan**, R.R. Hark, D. Kuck

ORGN 510. Measuring the relative strength of intramolecular OH/OH bonds through equilibrium isotope effects (EIEs). **K. Kolahdouzan**, O. Ogba, D.J. O'Leary

ORGN 511. Study of the tunneling-ready-state electronic structures in hydride versus deuteride transfer reactions. **N. Salimraftar**

ORGN 512. Conformational dependence of the mechanism of Michael addition of enones to guanine. **C. Paquin**, D.W. Boerth, V. Sammeta

ORGN 513. Testing the isotopically different tunneling-ready-state conformational and electronic structures in hydride transfer reactions. **L. Ma**, Y. Lu

ORGN 514. Advances in the development of redox-active organic molecules as anolytes for grid-scale energy storage. **M.E. Cook**, J. Ruchti, M.S. Sanford, M.S. Sigman, S.D. Minteer

ORGN 515. Empirical and computational studies drive complete understanding of the mechanism of silane-mediated reductions of phosphine oxides. **K. Wang**, J. Buonomo, C.C. Aldrich

ORGN 516. Computational study of heavy-atom tunneling in the Möbius pi-bond shifting in [4n]- and [4n+2] annulenes. **C.S. Michel**, **J. Arbitman**, C. Castro, W.L. Karney

ORGN 517. Primary isotope dependence of the secondary kinetic isotope effects and Hammett correlations in hydride transfer reactions in solution. **S.N. Wilhelm**, P. Rahmani, C. Hall, Y. Lu

ORGN 518. Computational investigation of conical intersections in the photofragmentation of arylmethyl and arylallyl acetates. **T.C. Celius**, B.K. Carpenter

ORGN 519. Competing triplet state [2+2] photodimerization in the solid state using naphthoquinone derivatives. **K. McKay**, D. Shields, S.K. Sarkar, J.A. Krause, A.D. Gudmundsdottir

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

ACS Award for Creative Work in Synthetic Organic Chemistry: Symposium in honor of Brian M. Stoltz

‡*Cooperative Cosponsorship*

R.D. Broene, *Organizer*
N.K. Garg, *Presiding*

8:00 Introductory Remarks.

8:05 ORGN 520. Necessity is the mother of invention: Natural products and the chemistry they inspire. **S.E. Reisman**

8:45 ORGN 521. Total synthesis of (±)-phomoidride D: A 22 year odyssey. J. Leung, A. Bederman, J.T. Njardarson, D.A. Spiegel, G. Murphy, N. Hama, T. Shirahata, B.M. Twenter, P. Dong, I. McDonald, M. Inoue, N. Taniguchi, T. McMahon, N. Tao, C. Schneider, B.M. Stoltz, **J.L. Wood**

9:25 ORGN 522. Catalytic C–H insertion reactions of phenyl carbocations. **H. Nelson**

10:05 ORGN 523. Strategies and methods for chemical synthesis inspired by natural products. **R. Sarpong**

10:45 Introduction of Awardee.

10:50 ORGN 524. Award Address (ACS Award for Creative Work in Synthetic Organic Chemistry Sponsored by MilliporeSigma). Complex natural products as a driving force for discovery in organic chemistry. **B.M. Stoltz**

Section B
Ernest N. Morial Convention Center
R02

National Fresenius Award: Symposium in honor of Thomas J. Maimone

S.M. Silverman, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN 525. New strategies and methods in the synthesis of natural products. **S. Pronin**

8:50 ORGN 526. Synthesis of complex anticancer alkaloids and terpenes. **D. Sarlah**

9:35 ORGN 527. Total synthesis of neurologically active terpenoid natural products. **T.R. Newhouse**

10:20 ORGN 528. Electrophilic heteroatom rearrangements with N-ligated hypervalent iodine reagents: Synthesis of medium-ring oxygen heterocycles. **S. Wengryniuk**

11:05 Introduction of Awardee.

11:10 ORGN 529. Award Address (National Fresenius Award Sponsored by the Phi Lambda Upsilon, The National Chemistry Honor Society). Synthesis of complex terpenes from simple precursors. **T.J. Maimone**

Section C
Ernest N. Morial Convention Center
R01

Heterocycles & Aromatics

R.D. Broene, *Organizer*
J. Li, *Presiding*

8:00 ORGN 530. Transannular cyclization and Iodoacetoxylation approaches to heterocycle peptidomimetics. **W.D. Lubell**, N. Atmuri

8:20 ORGN 531. Synthesis of chiral nitrogen heterocycles via carbonyl-olefin metathesis. **E.J. Groso**, B.W. Alexander, C. Schindler

8:40 ORGN 532. Synthesis of functionalized pyrazoles *via* copper-catalyzed *C-N* dehydrogenative cross-coupling for prostate cancer therapy by inhibiting tubulin polymerization. **D. Sar**, S.K. Misra, I. Srivastava, D. Pan

9:00 ORGN 533. Synthesis of enantioenriched Isoindolines and dihydropyrroles via intramolecular hydroamination of sulfonamides. **Y.O. Tao**

9:20 ORGN 534. Novel synthesis of benzo[*b*]thiophenes, thiophenes, and selenophenes using sodium salts. **C.A. Walter**, N. Fallows, **T. Kesharwani**

9:40 ORGN 535. Synthesis of diverse benzo[b]thiophene derivatives via iodine mediated one-pot successive cyclization-alkylation reaction strategy. **C. Cunningham**, K. Whalen, S. Khan, T. Kesharwani

10:00 ORGN 536. Exploring the decarboxylative cross-coupling of biomass carbohydrates derived furans to obtain value-added platform chemicals. **P. Forgione**

10:20 ORGN 537. Mechanochemical synthesis of porphyrins with bulky *meso*-substituents. **T.D. Hamilton**, Q. Su, D. Cordero

10:40 ORGN 538. cis-Specific synthesis of 1,3-disubstituted tetrahydro-β-carbolines from N-sulfonyl N,S-acetals. **J. Li**, S. Luo, Y. Liu, D.F. Ortwine, J. Zbieg, J. Liang, X. Wang

Section D
Ernest N. Morial Convention Center
R04

CH Activation

R.D. Broene, *Organizer*
E.J. Phipps, *Presiding*

8:20 ORGN 539. Rhodium-catalyzed intermolecular C–H functionalization as a key step in the synthesis of complex stereodefined arylpyrrolidines. **R.W. Kubiak**, H.M. Davies

8:45 ORGN 540. Catalyst-controlled enantioselective, diastereoselective and site-selective functionalization of unactivated C-H bonds. **W. Liu**, H.M. Davies

9:10 ORGN 541. Computational studies on gold(I)-catalyzed outer sphere functionalizations of C(sp^3)-H bonds. **V. Gandon**

9:35 ORGN 542. Cobalt-catalyzed directed functionalization of sp^2 C-H bonds. **T. Nguyen**, O. Daugulis

10:00 ORGN 543. Thioether-palladium catalysis for efficient oxidative heteroarene C–H functionalization. **L. Wang**, B. Carrow

10:25 ORGN 544. Rh(III)-catalyzed diastereoselective cyclopropanation of allylic alcohols initiated by C–H activation. **E.J. Phipps**, T. Piou, T. Rovis

10:50 ORGN 545. Catalytic δ-C(sp^3)–H silylation of alcohols. **A. Bunescu**, T. Butcher, J.F. Hartwig

11:15 ORGN 546. Copper-mediated domino C-H iodination and nitration of indoles. **C. Jiang**, D. Tu

11:40 ORGN 547. Ligand-promoted rhodium(III)-catalyzed *ortho*-C–H functionalization. **Y. Lu**

Section E
Ernest N. Morial Convention Center
R05

Total Synthesis of Complex Molecules

R.D. Broene, *Organizer*
R. Rafferty, *Presiding*

8:20 ORGN 548. Total synthesis and biological evaluation of new complex alkaloids. **A.H. Antropow**, M. Movassaghi

8:40 ORGN 549. Divergent total syntheses of (±)-alstoscholarisines B and C. **J.D. Mason**, S.M. Weinreb

9:00 ORGN 550. Enantioselective total syntheses of akuammiline alkaloids. **L. Morrill**, N.K. Garg

9:20 ORGN 551. Total synthesis of Gelsemium alkaloids via a metal-catalyzed cycloisomerization. **P. Knutson**, E.T. Newcomb, B. Pedersen, E. Ferreira

9:40 ORGN 552. Total synthesis of the alkaloid antibiotic berberine. **A. De Los Santos**, L.M. Mori Quiroz, M.D. Clift

10:00 ORGN 553. Synthetic efforts towards brocazine F & G: Total synthesis and new chemical screening libraries. **W.W. Hulangamuwa**, C. House, R.J. Rafferty

10:20 ORGN 554. Catalyst-controlled oligomerization for the synthesis of polypyrroloindoline natural products. **J. Lipshultz**, D.W. MacMillan, J.J. Badillo, R.J. Comito, C. Jamison

10:40 ORGN 555. Progress towards the total synthesis of parviflorene A, F and G. **M.R. Becker**, K. Rykaczewski, C. Schindler

11:00 ORGN 556. Synthetic studies on the bis-guanidinium toxins 11-saxitoxinethanoic acid and zetekitoxin AB. **D.T. Tang**, J.E. Merit, J. Du Bois

11:20 ORGN 557. Lagunamide C: Efforts in total synthesis, biological evaluation, and drug delivery. **R. Rafferty**, A. Fatino, C. Hanks, Y. Zhang, J. Dallman, K. Eschliman

Section F
Ernest N. Morial Convention Center
R03

New Reactions & Methodology

R.D. Broene, *Organizer*
O. Larionov, *Presiding*

8:40 ORGN 558. Functionalization of allylic alcohols via a radical relay chaperone strategy. **K. Nakafuku**, S. Fosu, D.A. Nagib

9:00 ORGN 559. Radical-chaperone mediated C–H mono- and di-halogenation of alcohols. **E. Wappes**, A. Vanitcha, D.A. Nagib

9:20 ORGN 560. Rapid access to diverse oxazoles via radical C-H amination. **A. Chen**, D.A. Nagib

9:40 ORGN 561. Photocatalytic prenylation of perfluoroarenes. **S. Priya**, J.D. Weaver

10:00 ORGN 562. Development of selective photoinduced transformations for organic synthesis. **O. Larionov**

10:20 ORGN 563. Merging photocatalysis & prenylation. **M. Rathnayake**, J.D. Weaver

10:40 ORGN 564. Withdrawn.

11:00 ORGN 565. Photo- and electrochemical methods for lignin valorization. **G. Magallanes**, I. Bosque Mart?nez, M. Riguolet, M.D. Karkas, C. Stephenson

11:20 ORGN 566. Visible-light-promoted C–S cross-coupling via intermolecular charge transfer. **B. Liu**, C. Lim, G. Miyake

Discovery of Small Molecules Targeting RNA: Where Are We & Where Are We Going?
Sponsored by MEDI, Cosponsored by CARB and ORGN

Recent Advances in Catalytic Carbohydrate Reaction Development
Sponsored by CARB, Cosponsored by ORGN

WEDNESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
La Nouvelle Orleans Ballroom C

Ernest Guenther Award in the Chemistry of Natural Products: Symposium in honor of David R. Williams

C.A. Maryanoff, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN 567. Reaction cascades for building complex carbocycles and heterocycles from simple precursors. **A.J. Frontier**

1:55 ORGN 568. Total synthesis of complex natural products. **S. Herzon**

2:45 ORGN 569. Vinblastine: Synthetic and mechanistic studies. **D.L. Boger**

3:35 Introduction of Awardee.

3:55 ORGN 570. Award Address (Ernest Guenther Award in the Chemistry of Natural Products Sponsored by Givaudan). Significance of strategy and the origins of discovery in organic synthesis. **D.R. Williams**

4:55 Concluding Remarks.

Section B
Ernest N. Morial Convention Center
R02

Flow Chemistry & Continuous Processes

‡*Cooperative Cosponsorship*

R.D. Broene, *Organizer*
S.K. Collins, *Presiding*

1:00 ORGN 571. Reaction scale up using flow chemistry in a stereoselective aldol/epoxidation reaction. **J.A. Hansen**, D. Bell, K. Ruark, Y. Sawyer

1:20 ORGN 572. Photochemical dual-catalytic synthesis of alkynyl sulfides. **J. Santandrea**, C. Minozzi, C. Cruché, S.K. Collins

1:40 ORGN 573. On-site on-demand continuous processing: Cyanogen bromide and other chemical generators. **C. Kappe**

2:00 ORGN 574. *In-situ* on-demand production of anhydrous diazomethane using membrane separation technology. **D. Dallinger**, C. Kappe

2:20 ORGN 575. Preparation of polysubstituted cyclopropane derivatives using continuous flow synthesis of alkyl-substituted diazomethane. **A.B. Charette**, P. Rullière, E.M. Allouche, G. Benoit

2:40 ORGN 576. Photochemical intramolecular amination for the synthesis of heterocycles. **S. Parisien-Collette**, C. Cruché, X. Abel-Snape, S.K. Collins

3:00 ORGN 577. Extension of the GBBR: A green, robust, scalable and efficient continuous flow synthesis of fused 3-aminoimidazoheterocycles. **B. Baker**, W. Kerr, D. Poole

3:20 ORGN 578. Combinatorial surface chemistry via massively parallel solution nanophotochemistry. **D. Valles**, C. Carbonell, A.B. Braunschweig, A. Wong

3:40 ORGN 579. Continuous flow technology in the production of fine chemicals and APIs. **M. Movsisyan**, T. Heugebaert, B.I. Roman, R. Dams, C.V. Stevens

4:00 ORGN 580. Advances and opportunities in flow electrochemistry. **T. Wirth**

4:20 ORGN 581. Continuous flow diazotisation of amines. **C. Audubert**, H. Lebel

4:40 ORGN 582. Development of photochemical processes in continuous flow. **S.K. Collins**

Section C
Ernest N. Morial Convention Center
R01

Peptides, Proteins & Amino Acids

R.D. Broene, *Organizer*
M.W. Giuliano, *Presiding*

1:00 ORGN 583. Substrate specificity and mechanism of a class C radical SAM thiazole methyltransferase. **N. Mahanta**, Z. Zhang, g. hudson, W.A. Van Der Donk, d. mitchell

1:20 ORGN 584. nano-FTIR: Nanometer-scale near-field spectroscopy for probing protein secondary structure of individual protein complexes. **P. Schäfer**, T. Gokus

1:40 ORGN 585. Investigation of the solution conformations of macrocycles: Applications in the exploration of weak interactions and in drug design. **E. Danelius**, M. Erdelyi, H. Andersson, P. Jarvoll

2:00 ORGN 586. Combining Staudinger ligation and copper-catalyzed click reactions for the synthesis of heteromultivalent glycomimetics. **T. Freichel**, N.L. Snyder, L. Hartmann

2:20 ORGN 587. [azaPhe[4]]-GHRP-6 azapeptides as CD36 modulators. **W.D. Lubell**, K. Chignen Possi, M. Mulumba, S. Omri, H. Ong, S. Chemtob

2:40 ORGN 588. Driving the efficiency of sortase-mediated ligation through metal-peptide complex formation. **S. Reed**, D. Brzovic, J. Antos

3:00 ORGN 589. Optimization of stapled peptide inhibitors of the estrogen receptor/coactivator interaction. **T.W. Moore**, T. Speltz, C.G. Mayne, J. Danes, S. Fanning, B. David, G. Greene, J.M. Frasor

3:20 ORGN 590. Use of pre-PEGylated Fmoc-Lys and Gln in synthesis of PEGylated peptide analogs of peptide hormone drug candidates with branched or unbranched short, monodiserse PEGs. P. Hamilton, W.L. Weibley, V. Haberman, T.M. Chu, **M. Wetzler**

3:40 ORGN 591. Interplay of sequence and environment in the conformation of human neuropeptides. **M.W. Giuliano**

Section D
Ernest N. Morial Convention Center
R04

CH Activation

R.D. Broene, *Organizer*
F. Williams, *Presiding*

1:30 ORGN 592. Electrochemical C-H oxidation of heterocyclic compounds. **M. Dissanayake**, A.K. Vannucci

1:55 ORGN 593. Hydrocarbon C–H insertion reactions of phenyl cations enabled by weakly coordinating anions. B. Shao, **A.L. Bagdasarian**, S. Popov, H. Nelson

2:20 ORGN 594. Simple and clean trifluoromethylation and alkylation of aromatics enabled by light. W. Liu, L. Li, P. Liu, **C. Li**

2:45 ORGN 595. Carbon dioxide as a hybrid directing group for the C-H activation of aliphatic and aromatic amine substrates. **M. Young**

3:10 ORGN 596. Withdrawn

3:35 ORGN 597. Transition metal catalysed intermolecular C-H amidation of arenes. **P. Kilaru**, K. Das, P. Zhao

4:00 ORGN 598. Investigation of the direct arylation polycondensation of silole-thiophene-S,S-dioxide monomers. **S. Mckinnon**, A. Smith, C. Scott

4:25 ORGN 599. Inter- and intramolecular aryl insertion reactions of borylnitrenes. **F. Williams**

Section E
Ernest N. Morial Convention Center
R05

Total Synthesis of Complex Molecules

R.D. Broene, *Organizer*
D. Martin, *Presiding*

1:20 ORGN 600. Progress toward the synthesis of neuroprotective limonoids. **D.B. Martin**, T.J. Clay, T.S. Alexander

1:40 ORGN 601. Studies toward the total synthesis of vitisinol D and evaluation of its analogs as neuroprotective agents. **S. Maki**, W. Bollinger, K. Dawson-Scully, P. Maity, S.D. Lepore

2:00 ORGN 602. Biomimetic synthesis of halogenated meroterpenoids isolated from marine bacteria. **J. George**

2:20 ORGN 603. Efficient synthesis of 1,3-anti-diol containing bioactive natural products and corresponding analogs via modular, pot-economical and library amenable protocols. **S. Javed**, A. Ganguly, G.C. Dissanayake, P.R. Hanson

2:40 ORGN 604. Leveraging electrochemical oxidation for the synthesis of phenylpropanoid natural products. **K.J. Romero**, C. Stephenson

3:00 ORGN 605. Synthesis of aromatic belts from cycloparaphenylenes. **C. Colwell**, T. Schaub, R. Jasti

3:20 ORGN 606. Total synthesis of (–)-azaspiracid-3. **N. Kenton**, D. Adu-Ampratwum, C.J. Forsyth

3:40 ORGN 607. Biomimetic synthesis of homodimericin A and synthetic studies of *Swertia* natural products. D. Ma, P. He, Y. Liu, **Z. Wang**

4:00 ORGN 608. Studies toward the synthesis of Gnetin H. **S.T. Handy**

Section F
Ernest N. Morial Convention Center
R03

New Reactions & Methodology

R.D. Broene, *Organizer*
C. Yeung, *Presiding*

1:00 ORGN 609. Catalytic polarity-reversed couplings of ketyl radicals. **S.M. Rafferty**, L. Wang, J. Lear, D.A. Nagib

1:20 ORGN 610. Regiodivergent functionalization of steroids. M. Charaschanya, **J. Aube**

1:40 ORGN 611. Catalytic C–H amination of alcohols via radical relay chaperones. **L.M. Stateman**, E. Wappes, K. Nakafuku, D.A. Nagib

2:00 ORGN 612. Quantifying Lewis acidity and oxophilicity of Lewis acid metal-ligand complexes for asymmetric catalysis using ^{31}P NMR spectroscopy. **J. Jennings**, B.W. Wigman, B.M. Armstrong, A.K. Franz

2:20 ORGN 613. Hydrogen atom transfer from hydrosilanes by Lewis base catalysis. **P. Asgari**, J. Jeon, Y. Hua

2:40 ORGN 614. Understanding and developing reactivity using a data-intensive approach. **A. Christian**, Z. Niemeyer, M.S. Sigman, D. Toste

3:00 ORGN 615. 1,3-Amino alcohol synthesis via a catalytic 3-step cascade. **B. Pierce**, R.E. Whittaker

3:20 ORGN 616. Recent advances in silane reagent design. **J. Buonomo**, C.C. Aldrich

3:40 ORGN 617. Trimethylchlorosilane as water scavenger: 10 years after presentation on 235th ACS National Meeting in New Orleans. **D. Volochnyuk**, S. Ryabukhin

4:00 ORGN 618. Metal- and acid-free C–H formylation of nitrogen heterocycles. **C. Yeung**, J.M. Ganley, M. Christensen, Y. Lam, Z. Peng, A.R. Angeles

WEDNESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall B1

Heterocycles & Aromatics

S.M. Silverman, *Organizer*

7:00–9:00

ORGN 619. Synthesis of differentially substituted pyrido[3,4-b]indoles by Rh(I)-catalysis. **B. Saliba**, M. Gentile, K. Queenan, J. Song, S.P. Mulcahy

ORGN 620. Lewis acid mediated ring opening of 4-ethynyltetrahydrofuroisoxazolines to produce anticipated antimicrobial 5-a-halo-4-propargylicisoxazolines. **K.G. Stevens**, **C.J. Jensen**, J.L. Duffy-Matzner

ORGN 621. Iron-catalyzed one pot synthesis of quinazoliones from alcohols and o-aminobenzonitriles under aerobic condition. **Y. Hu**, B. Li

ORGN 622. Effect of benzofulvene's exocylic substitutions on conjugation and aromaticity. **C. Fisher**, **C. Whyte**, A. Glass

ORGN 623. Synthesis and reactivity of C-3 carbohydrate exo-cyclic enones. **H. Arcure**, R. Hohol, Z.J. Witczak, D.E. Mencer, R. Bielski

ORGN 624. Pyrrolidine ring formation through the Michael addition of haloethylamines to beta-nitrostyrenes. **S. Liang**, D.A. Hunt

ORGN 625. Study of the reaction of 1,2-cyclohexanedione with omega-N-BOC alkyl amines. **J. Kloskowski**, D.A. Hunt

ORGN 626. Synthesis and purification of highly substituted anthraquinones. **M. Stern**, J.J. Reczek

ORGN 627. Condensation reactions of 2-formylbenzoic acid with arenes catalyzed by Brønsted superacids. **T.H. Swihart**, B.N. Nguyen, E.R. Marinez

ORGN 628. Studies of the cyclization reactions of dimethoxyazetidine compounds. **R. Magee**, L.M. Bradley

ORGN 629. Rearrangement of N-methyl palladium(II) and rhodium(III) carbaporphyrins. **A. Latham**, T.D. Lash

ORGN 630. Strategies for the synthesis of azuliporphyrin dimers. **M.E. Metallo**, T.D. Lash

ORGN 631. Synthesis of spiro-containing

‡*Cooperative Cosponsorship*

1,4-oxazepines from *N*-propargylic β-enaminones. **E. Karadeniz**, Y. Kelgokmen, M. Zora

ORGN 632. Influence of 1,2,3-triazole aromaticity on electron spin distribution in annulenotriazole anion radicals. **S.J. Peters**, D.L. Maybell

ORGN 633. Investigations directed towards the synthesis of carbachlorins. **M.A. Noboa**, T.D. Lash

ORGN 634. Transition-metal-free and base-free electrosynthesis of 1*H*-substituted benzimidazoles. **M. Dissanayake**, A.K. Vannucci

ORGN 635. Expedient 'on water' chemoselective green synthesis of 4-aminocoumarin bearing chromeno[4,3-*b*]quinolin-6-ones. **D. Bandyopadhyay**, C. Pena, V.M. Cano

ORGN 636. Chemoselective concurrent synthesis of benzimidazoles and 1,2-disubstituted benzimidazoles: Greener route and *in vitro* anti-cervical cancer evaluation. **D. Bandyopadhyay**, D.R. Garcia, J. Cruz, E. Arredondo-Espinoza, F.E. Olazaran Santibanez, I. Balderas-Renteria

ORGN 637. Bipyridinium tetraester: An air stable radical cation. J. Richard, M. Berville, **C. Boudon**, J. Wytko, S. Choua, T. Baumgartner, M. Stolar, R. Laurent, J. Weiss

ORGN 638. Anchimeric assistance in reactions of *N*-allyl-4-alkylamino-1,8-naphthalimides. **C.J. Hartwick**, **L.E. Martinez**, A.K. Giebink, D.E. Lewis

ORGN 639. Tandem cyclizations of diynals catalyzed by copper(I): Cycloaromatizations via 5-endo cuprate additions to proximal alkynes. T.S. Hughes, **K.M. Allen**

ORGN 640. Preparation of fundamental building blocks of oligoviologens. **W. Hau**, A. Soltis, B. Harvey, K. Bradely, O.V. Morgan, D.W. Scott, R. Morgan

ORGN 641. Synthesis of the [3.1.0] amino acid fragment of a ketohexokinase inhibitor for the treatment of NAFLD/NASH. **H. Wisniewska**, D.P. Fernando, A.C. Smith, M.S. Dowling, A. Shavnya, A.S. Tsai, L. Samp, J. Mustakis

ORGN 642. Total synthesis of hippadine and pratosine: Intramolecular de Mayo photocyclization. **C.I. Ochoa**, D.E. Minter

ORGN 643. Development of a synthetic strategy for the preparation of various para-functionalized aromatic substituents on a tri-substituted quinoline as drug candidates for HIV-1 integrase inhibition. **J. Hume**, N. Jentsch, A. Hart, J.A. Pigza, J. Sun, J. Kessl, M.G. Donahue

ORGN 644. Microwave-assisted synthesis of nitrogen heterocycles from substituted cyclic sulfates. **J.A. Chastant**, O. Do, M.L. Trudell

ORGN 645. Magnetic anisotropy of rotationally hindered nitrosoarenes. **S.A. Kelley**, C.E. Owens, S. Reach, S.C. Blackstock

ORGN 646. Synthesis and evaluation of nitrogen heterocycles for the antimicrobial activity. **S. Murru**, **K. Tran**, R. Bista

ORGN 647. 1-methyl-3-iodo-7-azaindole derivative synthesis novelized. **A. Phillips**, K. Naran, T. Kesharwani

Section A
Ernest N. Morial Convention Center
Hall E

New Reactions & Methodology

S.M. Silverman, *Organizer*

7:00–9:00

ORGN 648. Two-round functionalization of pyrrolidine to synthesize unsymmetrically 2,5-disubstituted pyrrolidines. **H. Rong**

ORGN 649. Efficient diastereoselective halo alkene functionalization using thiourea organocatalysts. **P.N. Poindexter**, J.J. Kiddle

ORGN 650. Investigation of catalytic epoxidation of alkenes over magnetic ferrite nanoparticles. **F.Y. Fezouni**

ORGN 651. Catalytic epoxidation of olefins over metal oxide nanoparticles. **J. Al Habsi**

ORGN 652. Substitution of essential oils at the C'3 Site of cefotaxime to test antibiotic effectivness. **B. Hunt**, A. Maroney, S.A. Brouet

ORGN 653. Redox-triggered β-C-H functionalizations of pyrrolidin-3-ol. **C. Yi**

ORGN 654. Diastereo- and site-selective synthesis of 1,3-amino alcohols via azaallyl anion ring-opening of epoxides. **P.E. Daniel**

ORGN 655. Mechanochemistry, a useful tool for the chemist s tool kit – application in medicinal chemistry @ AbbVie. **H. Geneste**, E. Colson, F. Regner, S. Triebel

ORGN 656. Novel syntheses of (Z)-β-amino β-substituted-β,β-unsaturated amides via rearrangement- replacement and Suzuki reactions. **X. Liu**, Y. Han, Q. Lin

ORGN 657. π-Conjugated triazenes: Intermediates that undergo oxidation and substitution reactions. **H. Barragan Peyrani**, A. Bugarin

ORGN 658. Microwave-assisted hydrogenation of aldehydes and ketones using frustrated Lewis pairs. **E.M. Valentin**, L. Robertson, Y. Miao

ORGN 659. Synthetic studies of polymers from half-esters obtained by practical selective monohydrolysis reaction. J. Shi, **S. Niwayama**

ORGN 660. General method for 1,2-bis(arylthio)arene synthesis via aryne intermediate. M. Mesgar, **J. Nguyen-Le**, O. Daugulis

ORGN 661. Withdrawn

ORGN 662. Tethered-zwitterionic-1,3-diaza-Claisen rearrangements of *in-situ* generated carbodiimides afford highly-substituted cyclic guanidines. **M. Luedtke**, J.D. Walker, J. Madalengoitia

ORGN 663. Preparation, structure, and reactivity of new (dichloroiodo)pyridines. **C.L. Makitalo**, **M. Jarvi**, K.D. Chau Nguyen, A. Yoshimura, V. Nemykin, V.V. Zhdankin

ORGN 664. Oxidative heterocyclization of aldoximes with heterocyclic alkenes mediated by hypervalent iodine reagent. **M. Shea**, K.D. Chau Nguyen, G. Rohde, M. Yusubov, **A. Yoshimura**, V.V. Zhdankin

ORGN 665. Copper-catalyzed hydroamination of heterocyclic amines to vinyl arenes. **S. Park**, S. Kang, Y. Lee

ORGN 666. Novel method for synthesis of allenes through copper-catalyzed propargylic reduction using *N*-heterocyclic carbene. **Y. Kim**, S. Park, Y. Lee

ORGN 667. Transition-metal free, visible-light-promoted C–S cross-coupling reaction. **B. Liu**, C. Lim, G. Miyake

ORGN 668. Halogenation of β-trimethylsilyl-β,β-unsaturated esters. **L.M. Fealy**, M.P. Jennings

ORGN 669. Stereoselective arylative-cyclopropanation process and selective carbon-phosphorus bond formation on anilines. **E. Deruer**, S. Canesi, S. Coulibali

ORGN 670. Purine nucleosides with reactive β-halovinyl and β-keto sulfones at C8 position. **A. Howlader**, S. Suzol, K. Blanco, S.F. Wnuk

ORGN 671. Parallel synthesis of piperazine-based small molecules for fragment-based drug discovery. S. Chamakuri, **K. Tran**, P. Jain, S. Guduru, C. Santini, D.W. Young

ORGN 672. Effect of proximal functionality on the allylic azide equilibrium. **J. Cox**, M.H. Packard, V. Suding, J. Topczewski

ORGN 673. Direct synthesis of 1,2-disulfonyl diazetidine derivatives and their synthetic applications. **J. Istre**

ORGN 674. Biomimetic haliranium-induced polyene cyclizations. **A.M. Arnold**, A. Pothig, T. Gulder

ORGN 675. Nexus of food, energy, and bioactivity: Tomato juice mediated, microwave-assisted green route towards bioactive pyrroles. **D. Bandyopadhyay**, L.M. Salinas, A. Ahmad

ORGN 676. Synthesis of naphthalenes via [4 + 2] cycloaddition of conjugated dienes and 2-pyrones with benzyne. **A. Dubrovskiy**, **M. Scotka**, **G. Jerezano**

ORGN 677. Development of hypervalent iodine guided electrophilic substitution (HIGES) reactions. **L. Dave**, C. Mowdawalla, I. Hyatt

ORGN 678. Novel Cu-catalyzed one-pot synthesis of 2-arylthiochromenones: Advantages of leaving group as an *in-situ* reagent. **S. Subramani**, S. Govindasamy

ORGN 679. Catalytic chalcogenylation under greener conditions: A regioselective, metal- and solvent-free, synthesis of 3-Se/S-indole/imidazo[1,2-a]pyridines catalysed by KIO_3. **A.L. Braga**, J. Khan, S. Saba

ORGN 680. Trifluoromethyl-β^6-tetrafluorosulfanyl-substituted two-carbon building blocks: New tools for the introduction of polar hydrophobicity. **N. Breen**, A. Ikeda, T. Tarasevich, J.T. Welch

ORGN 681. Metal-free chemoselective amide reductions utilizing novel Lewis acidic boron catalysts. **M. Peruzzi**, M.R. Gagne, S.J. Lee

ORGN 682. Titanium-mediated diastereoselective halo-aldol reactions resulting in β-vinyl β-hydroxy esters. **S. Maki**, P. Maity, S. Dougherty, J. Johns, S.D. Lepore

ORGN 683. Developing strategies for stilbene oligomerization based on persistent radical intermediates. **M.S. Galliher**, C. Stephenson

ORGN 684. Use of *N*-heterocyclic phenols as components in Ugi-Smiles Diels-Alder reactions. **N. Raeofy**, S. Luesse

ORGN 685. Study of regioselective House-Meinwald rearrangement (HMR) of spiro-epoxides. **N. Jeedimalla**, S. Roche

ORGN 686. Reactions of hypervalent iodonium alkynyl triflates with toluenesulfonylmethyl isocyanide (Tos-MIC). **M.E. Medard**, N. David, I.D. Hyatt

ORGN 687. Mechanistic investigation of reactions of bismuth(III) acetylides with organic azides in the copper(I)-catalyzed cycloaddition reaction. **A.L. Nazarova**, V.V. Fokin

ORGN 688. Rapid solution-phase synthesis of peptoids on gram-scale. B.C. Gorske, **S. Conwell**, **S. DeCarlo**, **J. Sharland**

ORGN 689. Exploration of Ugi-Smiles reactions involving oxy-Michael additions. **M. Zangi**, S. Luesse

ORGN 690. S_N1 alkylation of *C*-nucleophiles in aqueous mixtures: Effect of surfactant. **C. Ballard**

ORGN 691. Synthesis of polybrominated dibenzo-p-dioxins and mixed bromo/chloro dibenzo-p-dioxins. **A. Singh**, H. Hakk, S.J. Lupton

ORGN 692. Withdrawn

ORGN 693. Synthesis of heteroarylated steroid derivatives through an acid-catalyzed addition and dehydration sequence. T. Metz, **G. Lutovsky**, L.M. Stanley

ORGN 694. Disilanes as an alternative silicon source for copper-catalyzed silylations. **R. Van Hoveln**, B.J. McCarty, B.M. Thomas, T.S. Carpenter, S. Harruff, W.L. Kirkman

ORGN 695. Photoinduced synthesis of thiazolines. **M.E. Michaud**, P.D. Parker, J.G. Pierce

ORGN 696. New reactions of strained allylsilacycles. **E.J. Cummins**, G.W. O'Neil

ORGN 697. Radical relay strategy for β C–H amination of alcohols. **K. Nakafuku**, E. Wappes, D.A. Nagib

ORGN 698. Direct synthesis of *N*-(1-alkoxyvinyl)ammonium salts, an unusual class of *N*-quaternized ketene *N,O*-acetals. **A.M. Blades**, **D.L. McConnell**, **J.C. Sonberg**, D. Gomes Rodrigues, P.V. Keyes, C.F. Sullivan, O.M. Simone, J.D.

‡*Cooperative Cosponsorship*

Shapiro, B.C. Schafer, C.C. Williams, S. Rachad, C.E. Anthony, J.A. Goodman, M.M. Majireck

ORGN 699. C-H functionalization of alcohols: A single-electron strategy for molecular diversification. **E. Wappes**, A. Vanitcha, D.A. Nagib

ORGN 700. Synthesis of amino acids via catalytic C–H functionalization of alcohols. **L.M. Stateman**, E. Wappes, K. Nakafuku, D.A. Nagib

ORGN 701. Redox-neutral aldehyde couplings. **S.M. Rafferty**, L. Wang, J. Lear, D.A. Nagib

ORGN 702. Synthesis of fluorescent chromone and coumarin derivatives and their application as lead sensors and cell imaging agents. **J.R. Zimmerman**

ORGN 703. Radical coupling of feedstock alcohols and nitriles to access a library of oxazoles. **A. Chen**, D.A. Nagib

ORGN 704. Solvate ionic liquids as green alternatives for molecular solvents. **D. Eyckens**, L.C. Henderson

ORGN 705. Buchwald-Hartwig amination of aryl halides using solid-phase primary and secondary amines. **A. Rajewski**, **M. Embury**, J. Turk

Section A
Ernest N. Morial Convention Center
Hall E

Peptides, Proteins & Amino Acids

S.M. Silverman, *Organizer*

7:00–9:00

ORGN 706. Methionine oxidation leads to novel cross-links in peptide sequences containing methionine and histidine. **I. Prajapati**, O. Mozziconacci, C. Schoneich

ORGN 707. Progress toward a novel synthesis of a glycosylated asparagine residue. **K. Rykaczewski**, **L. Griggs**, J.M. Langenhan

ORGN 708. Conformational properties of *N*-vinyl and alkynyl substituted aromatic amides compounds. **R. Yamasaki**, K. Morita, A. Ito, K. Fukuda, I. Okamoto

ORGN 709. Employing the MeDbz linker to access C-terminally elongated peptides. **R. Stamatin**, C. Arbour, J.L. Stockdill

ORGN 710. Withdrawn

ORGN 711. Synthesis, characterization, and application of an unnatural boron and nitrogen containing isostere of tryptophan. **K.L. Boknevitz**, S.Y. Liu

ORGN 712. Potential anticancer depsipeptidic HDAC inhibitors accessed via an optimized solid-phase synthetic approach. **S.H. Smilen**, **E.M. Smith**, **P.A. Banks**, R.B. Fresco, C.T. Herr, R.T. Davison, **J.S. Miller**

ORGN 713. Asymmetric syntheses of conformationally constrained vinylogous β-amino acids and their incorporation into mixed backbone oligomers. **H. An**, H. Wu, T.J. Kodadek

ORGN 714. Optimizing the enzyme-like reactivity of a bifunctional helical peptide catalyst. **M.J. Campbell**

‡*Cooperative Cosponsorship*

ORGN 715. Proximity-enabled dual catalysis on a bifunctional helical peptide catalyst. **E.S. Weir**, D. Michaelis, M. Kinghorn

ORGN 716. Synthesis of methyl 1*H*-pyrazole-4-carboxylates bearing azetidine, pyrrolidine or piperidine substitutents on the heteroaromatic ring. **A. Sackus**, F.A. Sløk, G. Ragaite, J. Kuginyte, V. Malinauskiene, A. Kveselyte, G. Matuleviciute, V. Krisciuniene

ORGN 717. Design and synthesis of novel unnatural amino acids and their application in creating antibiotic polypeptides. W. Sams, S. Horiuchi, B. Rich, **K.A. Brien**, R. de la Salud Bea

ORGN 718. Synthesis of mutated peptides and computational evaluation of the FNII domain of the PLA_2R antigen in idiopathic membranous nephritis to determine the epitope regions. **S. Horiuchi**, Z. Parkinson, C. Welsh, S. Stoddard, **K.A. Brien**, R. de la Salud Bea

ORGN 719. Synthesis of mutated peptides and computational evaluation of the CTLD1 domain on the PLA_2R antigen in idiopathic membranous nephritis to determine epitope sites locations. **Z. Parkinson**, S. Horiuchi, C. Hayes, C. Welsh, S. Stoddard, R. de la Salud Bea, K.A. Brien

ORGN 720. Expanding the library of novel unnatural amino acids and their substitution in antibiotic polypeptides. **C. Drummond**, B. Rich, R. de la Salud Bea, K.A. Brien

ORGN 721. Synthesis of β,β-disubstituted amino esters: Expedient assembly of a library of fumimycin analogues. **S.S. Samanta**, S. Roche

ORGN 722. NMR and multivariate statistical study of the Maillard reaction of various sugars. **S. Lee**, J.A. Bjorklund

ORGN 723. Glycation reactions and their application towards ALS identification and treatment. **K. Lewis**, N.C. Tice, D.L. Smith

ORGN 724. Environment-dependent conformational behavior of endomorphin-1. **A.C. Schwartz**, S. Parnham, M.W. Giuliano

ORGN 725. Peptoid/thiopeptoid hybrids as polyproline type II helix mimics. **J. Sharland**, B.C. Gorske

Section A
Ernest N. Morial Convention Center
Hall E

Total Synthesis of Complex Molecules

S.M. Silverman, *Organizer*

7:00–9:00

ORGN 726. Synthesis of cyclic desmosines for elucidation of three dimensional structure of elastin. **D. Tokairin**, K. Ogawa, T. Hayashi, T. Usuki

ORGN 727. Synthesis of terpenoid cores in two steps. **E. Fereyduni**, G. Gonzalez, A.J. Grenning

ORGN 728. Analog oriented synthesis of terpenoid cores: toward dolestane and pseudo-guaianolide architectures. **F. Emmetiere**, A.J. Grenning

ORGN 729. Synthesis, anticancer and antileishmanial evaluation of β-phenyl acetylenic fatty acids and analogs. **C. Morales Guzman**, E. Álvarez Benedicto, Z. Torres Martínez, K. Griebenow, R. Balaña Fouce, N.M. Carballeira

ORGN 730. Progress toward the total synthesis of 11-demethoxymyrtoidine and myrtoidine. **A.M. Kazerouni**, D.E. Mancheno, E.S. Andreanksy, S. Blakey

ORGN 731. Synthetic study of anti-trypanosomal cynaropicrin. **T. Uchiyama**, T. Nakamura, T. Mori, S. Yamaguchi, D.B. Pitna, Y. Yoshimoto, T. Usuki

ORGN 732. Design and synthesis of novel macrolide antibiotics as tools against resistant bacteria. **A. Sanchez**, I. Seiple, Z. Zhang, A.G. Myers

ORGN 733. Total synthesis of pyrophen and campyrones A-C. **K.P. Reber**, H. Burdge

ORGN 734. Steps towards the novel synthesis of pancratistatin-type analogs. **A.P. Montoya**

ORGN 735. Asymmetric total synthesis of the natural product avrainvilleol. **A. Wegener**

ORGN 736. Total synthesis of arylnaphthalene lactone natural products *via* Hauser-Kraus annulation and Suzuki-Miyaura cross-coupling reaction. T. Kim, K. Jeong, B. Hwang, Y. Kim, M. Nakata, **J. Ham**

ORGN 737. Synthesis of biological evaluation of phidianidine analogues as neuroprotective agents. **D. Laws**, D. King, I. Schroeder, K. Rohal, D. Williams, B. Wakefield

ORGN 738. Total synthesis of baulamycins, a new family of siderophore inhibitors. **G. Ernouf**, A. Steele, W. Wuest

ORGN 739. Withdrawn

ORGN 740. Withdrawn

ORGN 741. Total synthesis of clavatadine B by direct, early stage guanidinylation. **M.T. Davenport**, **J.A. Dickson**, **M.R. Johnson**, S. Chamberland

ORGN 742. Progress towards the enantioselective total synthesis of a novel metabolite from *Streptomyces venezuelae*. **M. Cunningham**, S. Ankisetty, M. Slattery, J.M. Rimoldi

ORGN 743. Progress towards the total synthesis of indole-containing natural products using organocatalytic conjugate addition. **S. Oleynichenko**, J. Shih, J. May

ORGN 744. New bioactive agent discovery: Divergent total synthesis. **R. Rafferty**

General Posters
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PHYS

Division of Physical Chemistry

M. Duncan, *Program Chair*

SUNDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory

Fundamental Properties of the Exact Density Functional

Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
M.P. Levy, *Presiding*

8:30 PHYS 1. Atoms and bonds in molecular electronic wave functions: An intrinsic analysis. **K. Ruedenberg**

8:50 PHYS 2. Summation by educated match: A new, powerful technique to sum divergent series. G. Álvarez, **H.J. Silverstone**

9:10 PHYS 3. Solving the Schrödinger equation of atoms and molecules with the free complement theory. **H. Nakatsuji**

9:30 PHYS 4. Chemical potential, chemical hardness, Fukui function and dual descriptor for interacting systems. **J.L. Gazquez**, M. Franco-Perez, A. Vela

9:50 Intermission.

10:10 PHYS 5. Charge-separation models from the fragment-Hamiltonian approach. **S. Valone**

10:30 PHYS 6. Density functional theory in parameter space and its application to dynamics in condensed phase. **S. Ghosh**

10:50 PHYS 7. Thermodynamical representation of density functional theory. **A. Nagy**

11:10 PHYS 8. Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. **W. Yang**

Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Surfaces & Materials

M. Caricato, P.H. Vaccaro, *Organizers*
B. Kahr, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 9. Structure sensitive chiral surface chemistry: Enantioselectivity on chiral surfaces. **A.J. Gellman**, P. Kondratyuk, M. Payne

9:15 PHYS 10. Chiral materials based on tetrathiafulvalene and metal dithiolene complexes. **N. Avarvari**

9:55 PHYS 11. Understanding spontaneous chiral crystallization. J.E. Carpenter, **M. Gruenwald**

10:15 PHYS 12. Circular differential scattering of plasmonic pinwheels. **K.W. Smith**, H. Zhao, W. Chang, P.J.

Nordlander, S. Link

10:35 Intermission.

10:55 PHYS 13. Chiral inorganic nanostructures. **N. Kotov**

11:35 PHYS 14. Investigations of natural and magnetically induced "chirality" via response theory methods. **S. Coriani**

Section C
Ernest N. Morial Convention Center
Room 221

Cold Molecules for Chemistry

Quantum Simulation & Material

K.B. Whaley, *Organizer*
K. Ni, *Organizer, Presiding*
8:30 Introductory Remarks.

8:35 PHYS 15. Laser cooling of polyatomic molecules. **J. Doyle**

9:05 PHYS 16. Quantum dipolar spin liquids and Floquet Hopf insulators. **N. Yao**

9:35 PHYS 17. Advances in the preparation of ultracold molecules: Towards a quantum gas of polar $^{23}Na^{39}K$ molecules and Zeeman slowing of laser coolable diatomic molecules. T. Schulze, T. Hartmann, K. Voges, A. Zenesini, M. Petzold, P. Kaebert, M. Siercke, **S. Ospelkaus**

10:05 Intermission.

10:25 PHYS 18. Cold molecules in a lattice: From quantum strings to chemical synthesis. **K. Hazzard**

10:55 PHYS 19. Quantum control of ultracold molecular samples. **H. Naegerl**

11:25 PHYS 20. Predictive electronic structure theory for small molecules. **T. Shiozaki**

11:45 PHYS 21. Molecular ultracold plasma: evolution from a Rydberg gas and arrested relaxation. **J.S. Keller**

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Functional Ionic Liquids & Applications

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
T.L. Greaves, *Presiding*

8:30 Introductory Remarks.

8:35 PHYS 22. Infrared spectroscopy studies of the hypergolic reaction and decomposition of a dicyanoborohydride ionic liquid. **A.E. Thomas**, S.D. Chambreau

8:55 PHYS 23. Chemistry and space propulsion applications of room-temperature ionic liquids. **S.D. Chambreau**, G.L. Vaghjiani, S. Schneider

9:15 PHYS 24. Azole-functionalized boranes: Bringing the tunability of ionic liquids to molecular systems. **R.D. Rogers**

9:35 PHYS 25. On the creation and chemistry of ionic liquids stable in air for months at 300°C. **J.H. Davis**, K.N. West, B. Rabideau, T.G. Glover, B. Siu, R.A. O'Brien, M. Soltani, C. Cassity, M. Vo, J. McCants, E.A. Salter, A. Wierzbicki, A.C. Stenson, J.L. McGeehee

10:10 Intermission.

10:25 PHYS 26. Porous ionic liquids: structures and dynamics. **S. Dai**

11:00 PHYS 27. Porous liquids from metal organic frameworks in ionic liquids. **M. Costa Gomes**, L. Pison, C. Cervinka, A. Padua

11:35 PHYS 28. Solvent extraction in ionic liquids: Structuration and aggregation effects on extraction mechanisms. **S. Dourdain**, T. Sukhbaatar, G. Arrachart, S. Pellet-Rostaing

Section E
Ernest N. Morial Convention Center
Room 223

Energy & Charge Transfer at Nanoscale Interfaces

Interfaces in Electrochemistry & Catalysis

L. Huang, S.T. Roberts, K.A. Willets, *Organizers*
W. Chang, M.T. Sheldon, *Presiding*

8:30 PHYS 29. Exciton transport, coherent delocalization, auger annihilation and optical gain in 2D colloidal quantum wells. **T. Lian**

9:00 PHYS 30. From indirections find directions out. **M.A. Ratner**

9:30 PHYS 31. Ultrafast direct electron transfer at optoelectronic material interfaces. **W. Xiong**, B. Xiang, Y. Li, H. Pham, F. Paesani

10:00 PHYS 32. Surface electron dynamics in hematite (β-Fe_2O_3): Correlation between ultrafast surface electron trapping and small polaron formation. **L. Baker**, J. Husek, A. Cirri, S. Biswas

10:20 Intermission.

10:40 PHYS 33. Elucidating how photoexcited semiconductor nanocrystals drive redox catalysis. **G. Dukovic**

11:10 PHYS 34. Influence of surface-active molecules on reactions at liquid interfaces: Molecular dynamics studies. **I. Benjamin**, J.J. Karnes

11:40 PHYS 35. Controlling energy flow in plasmonic photocatalysis through the design of hybrid plasmonic nanostructures. **S. Linic**, U. Aslam, S. Chavez **12:00 PHYS 36.** Catalytic reactions on FeN_4/C site of Fe, N-functionalized carbon nanotubes as cathode catalyst for hydrogen fuel cells. **F. Gao**, G. Zhao, D. Bagayoko, D. Liu

Section F
Ernest N. Morial Convention Center
Room 224

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Cosponsored by COMP‡
M.S. Gordon, A. Krylov, R. Lindh, *Organizers*
T.L. Windus, *Organizer, Presiding*

8:30 PHYS 37. CI2030: The response to NSF's request for information on future needs for advanced cyberinfrastructure. **T.H. Dunning**

9:10 PHYS 38. Scientific evaluation of modern parallel programming models. **J.R. Hammond**

9:50 Intermission.

10:10 PHYS 39. Architecting science applications for exascale. **K. Riley**

10:50 PHYS 40. From legacy to exascale: GAMESS software development practices. **S.S. Leang**, M.S. Gordon

11:30 PHYS 41. Fast evaluation of scalar and vector fields of molecular properties on modern GPU and many-core architectures. **A. Vazquez-Mayagoitia**, R. Hernández-Esparza, J. Garza, R. Vargas

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms & Selectivity

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

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Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
Sponsored by POLY, Cosponsored by PHYS and PMSE

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL and PHYS

Chemistry of Molecular Electronics

Theory

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Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Data Mining & Frameworks for Chemical Discovery

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Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

SUNDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory
Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
J. Perdew, *Presiding*

1:30 PHYS 42. On the nature of the real part of the electron density and the resulting Fukui functions obtained from complex wave functions of temporary anion states. **R.C. Morrison**

1:50 PHYS 43. Renewed energy density concept as quantum mechanics 100 years of mystery is solved. **A. Tachibana**

2:10 PHYS 44. Pauli principle and the confinement of electron pairs In A symmetric double well potential. **P. Fuentealba**, T. Novoa, C. Cardenas

2:30 PHYS 45. Fluxional behavior and noble gas binding ability of boron clusters. **P. Chattaraj**

2:50 Intermission.

3:10 PHYS 46. The CsI band gap under strong compression. **A. Cedillo**

3:30 PHYS 47. Conceptual density functional theory: Applications in bonding, chemical reactivity and molecular design. **F.J. De Proft**

3:50 PHYS 48. Functional derivatives and differentiability in density-functional theory. **Y.A. Wang**

4:10 PHYS 49. Density functional reactivity theory: Its recent developments and applications. **S. Liu**

Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Linear Chiroptical Effects

M. Caricato, P.H. Vaccaro, *Organizers*
P.L. Polavarapu, *Presiding*

1:30 PHYS 50. Polarizing light with chiral supramolecular structures. **L. Di Bari**

2:10 PHYS 51. From isolated chiral molecule to the solid: Conformational study by laser spectroscopy and vibrational circular dichroism. **A. Zehnacker**

2:50 PHYS 52. Modeling solvent effects on chiroptical response properties with coupled cluster theory and implicit solvation. **J.C. Howard**, J.C. Womack, J. Dziedzic, C. Skylaris, T. Crawford

3:10 PHYS 53. Mechanical, electrical and magnetic anharmonicity in chiroptical vibrational spectra: The VPT2 approach. **J. Bloino**, A. Baiardi, F. Egidi, M. Fusè

3:30 Intermission.

3:50 PHYS 54. Vibrational circular dichroism spectroscopy as probe for intermolecular interactions. **C. Merten**

4:30 PHYS 55. Theoretical prediction of resonance Raman optical activity spectra. **J.R. Cheeseman**

Section C
Ernest N. Morial Convention Center
Room 221

‡*Cooperative Cosponsorship*

Cold Molecules for Chemistry

Quantum Computing

K. Ni, K.B. Whaley, *Organizers*
W. Campbell, *Presiding*

1:30 PHYS 56. Quantum information with molecular ions. **K. Brown**

2:00 PHYS 57. Quantum computation using arrays of N polar molecules. **S. Kais**, Z. Hu

2:30 PHYS 58. Ultracold molecular assembly. **J. Hood**, L.R. Liu, Y. Yu, J.T. Zhang, K. Wang, Y. Lin, T. Rosenband, K. Ni

3:00 Intermission.

3:20 PHYS 59. Quantum computing for quantum chemistry: An update from the trenches. **A. Aspuru-Guzik**

3:50 PHYS 60. Harnessing coordination chemistry for the construction of qubits. J.M. Zadrozny, M. Graham, C. Yu, M.S. Fataftah, **D.E. Freedman**

4:20 PHYS 61. Modifying conductivity and material properties of molecular ensembles under light-matter strong coupling. **G. Pupillo**

4:50 PHYS 62. Withdrawn

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Functional Ionic Liquids & Applications

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
R. Hayes, *Presiding*

1:30 PHYS 63. Choline-Amino Acid Based Ionic Liquids – From Solvent Structure to Lignin Dissolution. **H. Jiang**, G. Warr, R. Atkin, S. Imberti

1:50 PHYS 64. Ionic liquids as catalysists for biomass conversion. **K. Takahashi**

2:25 PHYS 65. Comparison of imidazolium- and cholinium-based ionic liquids for biomass pretreatment and "one-pot" conversion technologies. **B.A. Simmons**

3:00 PHYS 66. Pseudoprotic ionic liquids and protic mixtures: Strange cousins of ionic liquids. **M.N. Kobrak**

3:20 Intermission.

3:35 PHYS 67. High throughput and machine learning approaches to characterising stoichiometric and non-stoichiometric protic ionic liquid-water solutions. D. Yalcin, C. Drummond, **T.L. Greaves**

4:10 PHYS 68. Ionic liquid electrolytes for harvesting low-grade waste heat. **J. Pringle**, M. Dupont, A. Taheri, D. Al-Masri, D.R. MacFarlane

4:45 PHYS 69. A detailed study on thermophysical properties of natural deep eutectic solvents via combined experimental and theoretical approaches. S. Aparicio-Martinez, **M. Atilhan**

Section E
Ernest N. Morial Convention Center
Room 223

Energy & Charge Transfer at Nanoscale Interfaces

Emerging Techniques for Probing Nanoscale Structure & Dynamics

L. Huang, S.T. Roberts, K.A. Willets, *Organizers*
L. Baker, W. Xiong, *Presiding*

1:30 PHYS 70. Multimodal tip-enhanced spectroscopy. **M.B. Raschke**

2:00 PHYS 71. Chemically and structurally correlated carrier and exciton transport in solution-processed semiconductors. A. Hill, C.L. Kennedy, E. Massaro, **E. Grumstrup**

2:30 PHYS 72. Ultrafast two-dimensional infrared spectroscopy of disordered surfactant interfaces. C.P. Baryiames, E. Ma, **C.R. Baiz**

2:50 PHYS 73. Optical label- and model-free probe of the surface potential of nano and microscopic objects in aqueous solution. **S. Roke**

3:10 Intermission.

3:30 PHYS 74. Carrier dynamics in plasmonic nanostructures. **S. Link**

3:50 PHYS 75. Imaging the electronic structure of TIPS-pentacene microcrystals using two-dimensional white-light microscopy. **N.M. Kearns**, A.C. Jones, J. Ho, J.T. Flach, M.T. Zanni

4:10 PHYS 76. Femtosecond XUV transient absorption enables carrier- and element-specific measurement of interfacial charge transfer. **J. Vura-Weis**

4:30 PHYS 77. Understanding mislocalization error in plasmon enhanced super-resolution fluorescence microscopy. **H.J. Goldwyn**, D.J. Masiello

4:45 PHYS 78. Band-selective ballistic energy transport in oligomers characterized by relaxation-assisted 2D-IR spectroscopy. **L. Qasim**, Y. Yue, A. Kurnosov, A. Burin, I.V. Rubtsov

5:00 PHYS 79. Statistical mechanical modeling of excitons in condensed phases. **R. Remsing**

Section F
Ernest N. Morial Convention Center
Room 224

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Cosponsored by COMP‡
A. Krylov, R. Lindh, T.L. Windus, *Organizers*
M.S. Gordon, *Organizer, Presiding*

1:30 PHYS 80. Going from work station computing to exascale computing with the Dirac and Dalton programs. **H. Jensen**

2:10 PHYS 81. Scalability and programming productivity for massively-parallel wavefunction methods. **E. Solomonik**

2:50 PHYS 82. Tensor algebra systems for high-accuracy many-body formulations. **K. Kowalski**, B. Peng

3:10 Intermission.

3:50 PHYS 83. Toward reduced scaling many-body electronic structure at exascale. **E.F. Valeev**

4:30 PHYS 84. Numerical advances in finite temperature Green's function methods. **D. Zgid**, A. Rusakov, S. Iskakov

5:10 PHYS 85. Libtensor: General tensor contraction library for scientific computing on multiple platforms. **A. Krylov**

Section G
Ernest N. Morial Convention Center
Room 225

Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments

Spectra & Properties

H. Cuppen, D.E. Woon, *Organizers, Presiding*

1:30 Introductory Remarks.

1:35 PHYS 86. Accurate structure and spectroscopy of small molecular systems of astrophysical interest. T. Trabelsi, **J.S. Francisco**

2:10 PHYS 87. Quantum-chemical needs from the viewpoint of the Cologne Database for Molecular Spectroscopy. **H.S. Müller**

2:45 PHYS 88. Spectroscopic characterization of key aromatic and heterocyclic molecules: A route toward the origin of life. **C. Puzzarini**, V. Barone, J. Bloino, N. Tasinato

3:05 Intermission.

3:25 PHYS 89. Answering unique spectroscopic and astrochemical problems through quantum chemistry. **R.C. Fortenberry**, K.A. Kloska, J.P. Layfield, C.M. Novak, T.J. Lee

4:00 PHYS 90. Exploring the rotational and far infrared spectra of non-rigid species using highly correlated ab initio methods. **M.S. Senent**

4:35 PHYS 91. Infrared spectra of interstellar complex organic molecules: accurate energies and intensities by an anharmonic perturbative treatment. **J. Bloino**, A. Baiardi, C. Puzzarini, V. Barone

4:55 PHYS 92. Chocolate molecules in space: Utilizing tunable vacuum ultraviolet light for isomer specific detection of complex organic molecules from astrophysical ice analogues. **M. Abplanalp**, S. Góbi, A. Bergantini, A.M. Turner, R. Kaiser

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

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Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms at the Atomic Scale

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Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
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Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL and PHYS

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Artificial Intelligent Searching of Chemical Space

Sponsored by COMP, Cosponsored by CINF and PHYS

Chemistry of Molecular Electronics

Molecular-Scale Electronics

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Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

MONDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory

Conceptual Aspects

Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
M.F. Herman, *Presiding*

8:30 PHYS 93. On variational principles, and exact functional constraints, for ground states and excited states in time-independent density functional theory. **M.P. Levy**

9:00 PHYS 94. Adventures in density functional theory by a wavefunction theorist: A different, powerful perspective. **R. Bartlett**, D.S. Ranasinghe, Y. Park, P. Verma, Y. Jin, A. Perera

9:30 PHYS 95. Active space dependence of energy components and ingredients in multiconfiguration pair-density functional theory. **P. Sharma**, D.G. Truhlar, L. Gagliardi

9:45 Intermission.

10:00 PHYS 96. What Bob Parr has wrought: Quantum mechanics based reaction mechanisms for electrocatalysis. **W.A. Goddard**

10:30 PHYS 97. Where's my oscillator strength? **D.N. Beratan**

11:00 PHYS 98. Advances in orbital-free density functional theory simulations of materials. B. Gonzalez del Rio, W.C. Witt, J.M. Dieterich, **E.A. Carter**

11:30 PHYS 99. Nonlocal kinetic energy functionals by functional integration. **W. Mi**, A. Genova, M. Pavanello

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Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Nonlinear Effects

M. Caricato, *Organizer*
P.H. Vaccaro, *Organizer, Presiding*

8:30 PHYS 100. Novel chiroptical spectroscopies. **K. Ruud**

9:10 PHYS 101. From the theoretical predictions to the experimental demonstration of two-photon circular dichroism: "Uncovering the nonlinear optical property of chiral molecules". **F. Hernandez**

9:50 PHYS 102. Amplification of chirality in the enantioselective synthesis of intrinsically chiral terbium phosphate nanocrystals. **G. Markovich**, U. Hananel, A. Ben Moshe

10:10 PHYS 103. High-sensitivity time-resolved circular dichroism spectroscopy as a probe of structure and dynamics of strongly coupled artificial and natural molecular systems. **S. Savikhin**, V. Stadnytskyi, Z. Mitchell, G.S. Orf, R.E. Blankenship

10:30 Intermission.

10:50 PHYS 104. Electronic nonlinear spectroscopies: Theory and experiment working together. **A. Rizzo**

11:30 PHYS 105. Chiral sum frequency generation spectroscopy for protein characterization at interfaces. **E.C. Yan**

Section C
Ernest N. Morial Convention Center
Room 221

Cold Molecules for Chemistry

Cold Collisions & Dynamics

K. Ni, K.B. Whaley, *Organizers*
K. Hazzard, *Presiding*

8:30 PHYS 106. Slow-electron velocity-map imaging of cryogenically cooled anions (cryo-SEVI). **D.M. Neumark**

9:00 PHYS 107. Chemical reactivity at low temperatures: From potential energy surfaces to rate coefficients. **H. Guo**

9:30 PHYS 108. Collisions of ultracold NaRb molecules. **D. Wang**

10:00 PHYS 109. Universality and chaoticity in ultracold chemical reactions. **J.F. Croft**, C. makrides, M. Li, A. Petrov, B. Kendrick, B. Naduvalath, S. Kotochigova

10:20 Intermission.

10:50 PHYS 110. Four-center reactions of KRb molecules at sub microKelvin. **M. Hu**, Y. Liu, A. Gheorghe, Y. Lin, D. Grimes, K. Ni

11:10 PHYS 111. Molecules as reactive species at a collision energy close to absolute zero. **S. Kotochigova**

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Electrochemistry and Electrochemical Interfaces

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, J.F. Wishart, *Organizers*
S.K. Shaw, *Organizer, Presiding*

8:30 PHYS 112. Electrode-ionic liquids interfaces: Determination of the potential of zero charge and characterization of slower charging processes. **N.M. Vargas-Barbosa**, B. Roling

8:50 PHYS 113. Solvation dynamics of an ionic and a molecular probe in an ionic liquid and an deep eutectic solvent with similar structure. Y. Cui, **D.G. Kuroda**

9:10 PHYS 114. Electrochemistry and electrochemical processing in deep eutectic solvents. **K.S. Ryder**, A.P. Abbott, A. Hillman

9:45 PHYS 115. Tunable and stiff solid electrolyte made from an ionic liquid and a rigid-rod polyanion. **C. Zanelotti**, Y. Wang, S.E. Wollman, D. Yu, R. Kerr, M. Hegde, T.J. Dingemans, M. Forsyth, L.A. Madsen

10:05 Intermission.

10:20 PHYS 116. Magnetic control of ionic liquid ions in the electrical double layer. **R. Hayes**

10:55 PHYS 117. Viscosity dependent dynamics of electrochemically driven molecular reorientations revealed via vibrational spectro-electrochemistry. **A. Horvath**

11:15 PHYS 118. Directing bulk and interface interactions in ionic liquids to modulate ion solvation, conduction and structure in electrochemical systems. **B. Gurkan**, Q. Huang

11:35 PHYS 119. Ion diffusion in ionic liquids in electric fields. R.A. Clark, J. Edel, B. Kirchner, M.K. Kuimova, A.J. McIntosh, M.A. Nawawi, M. von Domaros, **T. Welton**

Section E
Ernest N. Morial Convention Center
Room 223

Energy & Charge Transfer at Nanoscale Interfaces

Materials for Photon Upconversion & Downcoversion

L. Huang, S.T. Roberts, K.A. Willets, *Organizers*
M.L. Tang, A. Willard, *Presiding*

8:30 PHYS 120. Resolving ultrafast exciton migration in organic solids at the nanoscale. S.B. Penwell, L.D. Ginsberg, R. Noriega, **N.S. Ginsberg**

9:00 PHYS 121. Manipulating energy and spin in hybrid organic-inorganic semiconductors. A.K. Le, J.A. Bender, A.P. Moon, R. Pandey, D.E. Cotton, E.K. Raulerson, B.A. Renard, **S.T. Roberts**

9:30 PHYS 122. Role of charge transfer states and vibronic coupling in singlet fission studied using 2D electronic spectroscopy. **A. Mandal**, M. Chen, E.D. Foszcz, R. Young, M.R. Wasielewski

9:45 PHYS 123. A generalized Ovchinnikov's rule can predict the biexciton boundedness in covalently linked singlet fission chromophores. V. Abraham, **N. Mayhall**

10:05 Intermission.

10:25 PHYS 124. Mechanisms of triplet pair separation and transport following singlet fission in functionalized pentacenes. **J.B. Asbury**

10:55 PHYS 125. Control of energy flow dynamics between photoactive ligands and semiconductor nanostructures. **J.C. Johnson**, M.C. Beard, J.E. Anthony, D. Kroupa, M. Martinez, D. Arias, J. Blackburn, M. Carroll

11:15 PHYS 126. Functional mode singlet fission theory. **H. Chen**

11:35 PHYS 127. Harvesting triplet excitons from intramolecular singlet fission. **F. Conrad-Burton**, F. Geyer, K. Miyata, C.P. Nuckolls, X. Zhu

11:50 PHYS 128. Aggregation induced vibrational displacements dominate excited state relaxation: Proposed singlet fission active polymers. **B. Datko**, D. Portlock, Z. Zhang, M. Williams, Y. Qin, R. Prasankumar, J.K. Grey

Section F
Ernest N. Morial Convention Center
Room 224

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Cosponsored by COMP‡
M.S. Gordon, R. Lindh, T.L. Windus, *Organizers*
A. Krylov, *Organizer, Presiding*

8:30 PHYS 129. Challenges in designing algorithms for quantum computers. **J.E. Rice**

9:10 PHYS 130. Exploring new architectures for computational chemistry. **S.V. Moore**

9:50 Intermission.

10:10 PHYS 131. Including energy usage considerations in quantum chemistry computations. **A.P. Rendell**, G. Mitre, A. Varghese, J. Milthorpe

10:50 PHYS 132. Vectorization and high performance quantum chemistry software. **E. Chow**, B. Pritchard

11:30 PHYS 133. Challenges in computing exact correlation energies: Reference functions and parallelization. **P.M. Zimmerman**

Section G
Ernest N. Morial Convention Center
Room 225

Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments

Spectra & Properties/Gas-Phase Collisions

H. Cuppen, *Organizer*
D.E. Woon, *Organizer, Presiding*
R.C. Fortenberry, *Presiding*

8:30 PHYS 134. Spectroscopic, theoretical, and observational study of aminomethanol, a predicted interstellar precursor to glycine. **S.L. Widicus Weaver**, B. Hays, M. McCabe, C. Powers, J. McMillan, S. Zinga

9:05 PHYS 135. Probing magnetic fields with methanol masers and ro-vibrational collision rates for modeling protoplanetary disks. **G.C. Groenenboom**, B. Lankhaar, A. van der Avoird

9:40 PHYS 136. Exploration of the structure and spectrum of CH_5^+ using diffusion Monte Carlo. **A.B. McCoy**, M.E. Fore

10:00 PHYS 137. Inorganic computational astrochemistry: Rovibrational quartic force fields. **N.J. Deyonker**, R.C. Fortenberry, Q. Cheng

10:20 PHYS 138. Diffuse interstellar bands and the pseudo-Jahn-Teller distortion in C_{60}^+. S. Ahmadvand, A.O. Lykhin, **S.A. Varganov**

10:40 Intermission.

11:00 PHYS 139. Computing collisional energy exchange: Theory, old and new, and comparison with experiments. **L. Wiesenfeld**

11:35 PHYS 140. Full-dimensional quantum dynamics of CO, CN, SiO, and CS in collisions with H_2. **B. Yang**, P. Zhang, C. Qu, P. Stancil, J.M. Bowman, B. Naduvalath, R. Forrey

12:10 PHYS 141. Mixed quantum/classical theory of molecular collisions: Applications to rotational-vibrational Inelastic scattering in astrophysical environmens. **D. Babikov**

Elucidation of Mechanisms & Kinetics on Surfaces

Theory

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Challenge & Opportunity in Lignin Valorization
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Applied Machine Learning: Molecular Dynamics, Materials & Virtual Screening

Sponsored by COMP, Cosponsored by CINF and PHYS

Chemistry of Molecular Electronics

Molecular-Scale Electronics

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Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Electrochemical Double Layer: Modeling, Characterization & Catalysis
Sponsored by CATL, Cosponsored by COMP, ENFL and PHYS

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MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory

Weak Interactions

Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
E. Gross, *Presiding*

1:30 PHYS 142. Optimized power series approximation for the correlation kernel for highly accurate and generally applicable Kohn-Sham methods based on the adiabatic-connection fluctuation dissipation theorem. **A. Goerling**, J. Erhard

2:00 PHYS 143. Following the path of Mel and John into the time-domain. **N.T. Maitra**

2:30 PHYS 144. Many body techniques for surface energies, interlayer binding energies and structural phase transitions. **A. Ruzsinszky**

3:00 PHYS 145. Generalized optimized effective potential for orbital functionals and self-consistent calculation of random phase approximations. **Y. Jin**, D. Zhang, Z. Chen, N. Su, W. Yang

3:15 Intermission.

3:30 PHYS 146. Single-particle excitation energies from the virial theorem. **A.D. Becke**

4:00 PHYS 147. Dreaming of banishing exact exchange: Semi local functionals as a key to understanding natural light harvesting? **S. Kuemmel**, T. Aschebrock, I. Schelter, T. de Queiroz

4:30 PHYS 148. Weight dependence of the exchange-correlation energy in ensemble density-functional theory. **E. Fromager**

4:45 PHYS 149. Reference determinant dependence of the random phase approximation in 3d transition metal chemistry. **J.E. Bates**, P. Mezei, G.I. Csonka, J. Sun, A. Ruzsinszky

5:00 PHYS 150. Improving the accuracy of inner shell excitation energies and reducing the self-interaction error with ionization potential optimized global hybrid functional. **Y. Jin**, R.J. Bartlett

5:15 PHYS 151. An introduction to projection functional theory: A method for finding excited states. **D.A. Engebretson**

5:30 PHYS 152. Low-lying excited states by constrained DFT. **P. Ramos**, M. Pavanello

Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Supramolecular Chirality

M. Caricato, P.H. Vaccaro, *Organizers*
C. Cappelli, *Presiding*

1:30 PHYS 153. Circular dichroism of multichromophoric biosystems: From structure to dynamics. **B. Mennucci**

2:10 PHYS 154. Host-guest complexes of chiral dimeric zinc porphyrin with achiral diamines: MC and MD simulations. **A.G. Petrovic**, B. Saha, S.P. Rath, N. Berova

2:50 PHYS 155. Exploiting induced chirality in supramolecular DNA assemblies. **M. Surin**

3:10 PHYS 156. Quantitative calculations of protein circular dichroism spectroscopy in the near-ultraviolet. **J.D. Hirst**

3:30 Intermission.

3:50 PHYS 157. Development and application of fragment-based methods for evaluating chiroptical spectra of large molecules. **K. Raghavachari**

4:30 PHYS 158. Simulating the selectivity of amino-acid based chiral selectors. **N.M. Cann**

Section C
Ernest N. Morial Convention Center
Room 221

Cold Molecules for Chemistry

New Cooling & Theoretical Techniques, Larger Molecules

K. Ni, K.B. Whaley, *Organizers*
E.R. Hudson, *Presiding*

1:30 PHYS 159. Direct cooling of polar molecules: Exploring a path to quantum degeneracy. **D. DeMille**, M. Steinecker, Y. Zhu, D. McCarron

2:00 PHYS 160. A strong, stimulated optical force for molecular deceleration. **W. Campbell**, X. Long, S. Yu, A. Jayich

2:30 PHYS 161. Many-body molecular dynamics: Enabling computer simulations with chemical and spectroscopic accuracy from the gas to the condensed phase. **F. Paesani**, P. Bajaj, M. Riera, O. Hamto, S. Brown

3:00 Intermission.

3:20 PHYS 162. High sensitivity microwave spectroscopy and molecular structure determination via cryogenic buffer gas cooling. **D. Patterson**

3:50 PHYS 163. O(^{3}P) + alkene chemistry in helium nanodroplets. **G.E. Douberly**

4:20 PHYS 164. Quantum dynamics of confined molecules. **P. Roy**

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Electrochemistry and Electrochemical Interfaces

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
K.S. Ryder, *Presiding*

1:30 PHYS 165. Local electric fields at the interfaces of ionic liquids and metals measured by Stark shift spectroscopy. J. Patrow, **J. Dawlaty**

1:50 PHYS 166. Electrode reactons in ionic liquids. **D.V. Matyushov**

2:25 PHYS 167. Withdrawn

3:00 PHYS 168. Ordered ionic liquid structure observed at terraced graphite interfaces by reflection high-energy electron diffraction. **D. Yang**, C. Wu, X. He

3:20 Intermission.

3:35 PHYS 169. Nitrogen reduction to ammonia in ionic liquids. **D. MacFarlane**

4:10 PHYS 170. Quasi-elastic and inelastic neutron scattering studies of glass-forming ammonium-based ionic liquids at low temperatures. **T. Lima**, Z. Li, M.C. Ribeiro, Y. Zhang

4:30 PHYS 171. Ion structure and dynamics in highly concentrated ionic liquid-alkali metal salt electrolytes. **M. Forsyth**, P. Howlett, F. Chen, D. MacFarlane

Section E
Ernest N. Morial Convention Center
Room 223

Energy & Charge Transfer at Nanoscale Interfaces

Energy Transfer in Biological & Synthetic Systems

L. Huang, S.T. Roberts, K.A. Willets, *Organizers*
C.R. Baiz, A. Mandal, *Presiding*

1:30 PHYS 172. Reducing energy losses and capitalizing on triplet-triplet annihilation at organic donor/acceptor interfaces. **B.P. Rand**

2:00 PHYS 173. Energetic disorder enhances exciton dissociation at the organic donor-acceptor interface. **A. Willard**

2:30 PHYS 174. Elucidating the energy and electron transfer dynamics in a self-assembled bilayer upconversion DSSC. **T. Dilbeck**, J. Wang, Y. Zhou, A. Olsson, K. Hanson

2:45 PHYS 175. Withdrawn

3:00 Intermission.

3:20 PHYS 176. Impact of the membrane-protein interface in photosynthetic light harvesting. **G. Schlau-Cohen**

3:50 PHYS 177. Synthetic biological control of quantum optical phenomena. A. Tsargorodska, G. Kodali, J. Mancini, L. Dutton, C. Hunter, P. Törmä, **G.J. Leggett**

4:10 PHYS 178. Exploring the multiscale design principles of excitation transport and light harvesting in the photosystem II membrane. **D. Bennett**, G.R. Fleming, K. Amarnath

4:25 PHYS 179. Bio-inspired energy conversion in non-equilibrium nano-systems: Electron-transfer coupled precipitation. **C. Kunstmann-Olsen**, M. Brust

4:40 PHYS 180. Understanding the structural evolution in 6,13-bis(triisopropylsilylethynyl) pentacene singlet fission through femtosecond stimulated Raman spectroscopy. **S. Kwang**, R.R. Frontiera

4:55 PHYS 181. Resolving inter-chromophoric coupling in tetrakis(perylene diimide) complexes. **D.J. Walwark**, Q. Wu, L. Yu, J.K. Grey

Section F
Ernest N. Morial Convention Center
Room 224

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Cosponsored by COMP‡
M.S. Gordon, A. Krylov, T.L. Windus, *Organizers*
R. Lindh, *Organizer, Presiding*

1:30 PHYS 182. New developments for matrix-product-state wave functions. **S. Knecht**

2:10 PHYS 183. Advances in the MADNESS parallel programming and numerical environment. **R.J. Harrison**

2:50 PHYS 184. Interoperability infrastructure in Psi4 and QCDB. **L.A. Burns**

3:30 Intermission.

3:50 PHYS 185. Charm++: Necessity of adaptive runtime systems for programming future parallel computers illustrated with NAMD and OpenAtom. **L. Kale**

4:30 PHYS 186. Highly parallel and large scale GW calculations within the OpenAtom software. **S. Ismail-Beigi**

5:10 PHYS 187. Spin-unrestricted second-order Møller–Plesset (MP2) forces for the condensed phase: Massively parallel implementation with application to the hydrated electron. **V. Rybkin**, J. Wilhelm, J. VandeVondele

Section G
Ernest N. Morial Convention Center
Room 225

Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments

Gas-Phase Reactions

H. Cuppen, *Organizer*
D.E. Woon, *Organizer, Presiding*
D. Talbi, *Presiding*

1:30 PHYS 188. High accuracy ab initio kinetics as a tool for astrochemistry. **S.J. Klippenstein**

2:05 PHYS 189. Nonadiabatic dynamics In warm dense matter and small molecules. **A.V. Akimov**

2:25 PHYS 190. State-of-the-art thermochemical and kinetic computations for complex organic molecules: Gas-phase formation routes in cold interstellar clouds. **V. Barone**, N. Tasinato, J. Bloino, D. Skouteris, C. Puzzarini

2:45 PHYS 191. Kinetic measurements of CO^+ and CO_2^+ reactions with N and O atoms for models of planetary atmospheres and the interstellar medium. J. Tenewitz, T. Le, S.G. Ard, N. Shuman, A.A. Viggiano, **J. Melko**

3:05 Intermission.

3:25 PHYS 192. Reaction mechanisms and rate constants of PAH growth in astrophysical environments. **A.M. Mebel**

‡*Cooperative Cosponsorship*

4:00 PHYS 193. Dynamics of pure and N-substituted cyclic aromatic hydrocarbon formation in the gas-phase. **P. Bera**, T. Stein, M.P. Head-Gordon, T.J. Lee

4:35 PHYS 194. Modelling dehydrogenation in interstellar PAHs. P. Castellanos, **A. Candian**, H. Linnartz, X. Tielens

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials

Frontal Polymerization

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Marriage of Machine Learning, Knowledge Representation & Chemical Sciences

Deep Learning for Deep Chemical Understanding

Sponsored by COMP, Cosponsored by CINF and PHYS

Chemistry of Molecular Electronics

Molecular-Scale Electronics

Sponsored by COLL, Cosponsored by PHYS

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
M.A. Duncan, *Organizer*

8:00–10:00

PHYS 195. Amino acid ionic liquids that selectively interact with proteins and lipid vesicles. G.A. Caputo, C. Wu, **T.D. Vaden**

PHYS 196. Coarse graining light-harvesting pendant assemblies to investigate the role of motion in energy transfer dynamics. **L. Bowers**, E. Puodziuknaite, J.R. Reynolds, J.M. Papanikolas

PHYS 197. Observation of the Marcus inverted region of electron transfer from asymmetric chemical doping of pristine (n, m) single-walled carbon nanotubes. **A.T. Liu**, Y. Kunai, M. Strano

PHYS 198. Photophysical studies of emerging organic/2D materials van der Waal heterostructures for plausible electronic applications. **A. Sarkar**, S.K. Pal

PHYS 199. Powering a CO_2 reduction catalyst with visible light through multiple subpicosecond electron transfers from a quantum dot. **S. Lian**, M. Kodaimati, E.A. Weiss

PHYS 200. Two-dimensional excitonic energy relaxation in carbon material revealed by ultrafast two-dimensional vibrational spectroscopy. **J. Wang**

PHYS 201. Direct imaging of ultrafast exciton transport in PCDTBT thin films by transient absorption microscopy. **E. Massaro**, A. Hill, C.L. Kennedy, E. Grumstrup

PHYS 202. Correlating singlet fission rate with intermolecular structure in perylenediimide thin films. **A.K. Le**, J.A. Bender, S.T. Roberts

PHYS 203. Water and proton concentration affects the electrocatalytic conversion of carbon dioxide in ionic liquids. **A. Hailu**

PHYS 204. Experimental determination of proton-cation exchange equilibrium constants fundamental to bioenergetics. H. Saeed, **J.W. Lee**

PHYS 205. Redox active deep eutectic solvents: proton-coupled electron transfer tuned two ways. **J.C. Goeltz**, P.J. Smith, L.N. Matsushima

PHYS 206. Reaction-diffusion model to describe the self organization of polycrystalline nanorods. **P. Knoll**, E. Nakouzi, O. Steinbock

PHYS 207. Interplay of ionic liquids and biomolecules: Considering protein structure and membrane permeability. **G.E. Lindberg**

PHYS 208. Synthesis of highly intense albumen-templated fluorescent nanoclusters using metal alloyed materials. **R. Jimenez**, S.P. Karna

PHYS 209. Probing protein-protein interactions in building blocks for supramolecular assemblies via SFG spectroscopy and MD simulations. **H.P. Hendrickson**, W. Liu, B. Rudshteyn, H. Wang, E.C. Yan, V.S. Batista

PHYS 210. Towards a better understanding of ion mediated DNA-surface interactions: Transition and alkaline earth metal ion interactions with a DNA duplex. **M. Provorse Long**, X. Liu, C. Isborn

PHYS 211. Proton motive force computation revealing latent heat utilization by localized protons at a liquid-biomembrane interface. **J.W. Lee**

PHYS 212. Operando imaging of the transient species from electron transfer at the biointerface. **X. Yu**

TUESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory

Strong Correlation

Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
K. Burke, *Presiding*

8:30 PHYS 213. SCAN density functional: Predictive power of 17 exact constraints. **J.P. Perdew**

9:00 PHYS 214. Structural and ferroelectric properties of prototypical ferroelectric materials: Comparative first-principles investigations. **Y. Zhang**, J. Sun, J.P. Perdew, X. Wu

9:15 PHYS 215. New semilocal density functional and its performance. **J. Tao**

9:45 PHYS 216. The strongly constrained and appropriately normed meta-generalized gradient approximation. **J. Sun**

10:15 Intermission.

10:30 PHYS 217. Recent advances in density functional theories. **D.G. Truhlar**

11:00 PHYS 218. Combinatorial design and assessment of a new double hybrid density functional. N. Mardirossian, **M.P. Head-Gordon**

11:30 PHYS 219. Interrogating the "B05" density functional for non-locality information. **S.G. Dale**, E.R. Johnson, A.D. Becke

Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Linear Chiroptical Effects

M. Caricato, P.H. Vaccaro, *Organizers*
J. Bloino, *Presiding*

8:30 PHYS 220. Applications of vibrational optical activity in pharmaceutical analysis. **L.A. Nafie**

9:10 PHYS 221. Fully polarizable embedding approach to chiroptical properties of aqueous solutions. **C. Cappelli**

9:50 PHYS 222. Investigating solvation effects on optical rotatory dispersion using the polarizable continuum model. **T. Aharon**, P. Lemler, P.H. Vaccaro, M. Caricato

10:10 PHYS 223. Unraveling intrinsic chiroptical properties: Cavity ring-down polarimetry of small organic molecules. **P. Lemler**, P.H. Vaccaro, C. Craft

10:30 Intermission.

10:50 PHYS 224. The use of chiroptical spectroscopy for identifying mis-identified chiral chemical structures. **P.L. Polavarapu**

11:30 PHYS 225. Non-covalent interactions in chiral molecular clusters: Chirality recognition/transfer/amplification. **Y. Xu**

Section C
Ernest N. Morial Convention Center
Room 221

Cold Molecules for Chemistry

New Chemistry Applications

K. Ni, K.B. Whaley, *Organizers*
J. Doyle, *Presiding*

8:30 PHYS 226. New tools to probe cold molecules and their interactions. **J. Ye**

9:00 PHYS 227. Rotationally inelastic scattering of HD (v=1, j=2) with H_2 or D_2 near 1 Kelvin. W.E. Perreault, N. Mukherjee, **R.N. Zare**

9:30 PHYS 228. Reaction dynamics and precision spectroscopy using cold samples of H_2 and He_2. M. Beyer, N. Hölsch, L. Semeria, P. Jansen, K. Höveler, J. Deiglmayr, **F. Merkt**

10:00 PHYS 229. Magnetic separation of water spin isomers in a molecular beam. **I. Braud**, J. Vermette, P. Turgeon, P. Ayotte, G. Alexandrowicz

10:20 Intermission.

10:40 PHYS 230. Probes of ion-neutral chemical dynamics with cold and controlled molecules. **S. Willitsch**

11:10 PHYS 231. Probing the internal temperature of cold trapped ion-molecule clusters. **E. Racow**, E. Castracane, S.E. Waller, Y. Yang, C.J. Johnson

11:30 PHYS 232. Low temperature quantum-state-resolved chemistry using physics tools. **E.R. Hudson**

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Computation, Theory & Simulation

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
S. Garrett-Roe, *Presiding*

8:30 PHYS 233. Large scale molecular simulations to interrogate nanostructuring and transport in transformational solvents for CO_2 capture. **V. Glezakou**, R. Rousseau, M. Nguyen, D.C. Cantu, D. Malhotra, D.J. Heldebrant, P. Koech, J. Page

8:50 PHYS 234. Role of quadrupolar interactions in the solvation of carbon dioxide in ionic liquids. **S. Corcelli**

9:25 PHYS 235. Structure in conventional and not so conventional aromatic ionic liquids. **K. Shimizu**, J. Canongia Lopes

10:00 PHYS 236. Mesoscale structural and dynamic correlations in ionic liquids sampled by atomistic molecular dynamics simulations. **D. Bedrov**, D. Dong, M. Ebrahiminia, J. Vatamanu

10:20 Intermission.

10:35 PHYS 237. What we learn from resolving dispersion and polarization interactions of ionic liquids. **A. Padua**

11:10 PHYS 238. Dynamical and dielectric properties of an ionic liquid using a charge transfer, polarizable model.

‡*Cooperative Cosponsorship*

S.W. Rick, C. Schroeder, A.S. Lyons

11:30 PHYS 239. Polarizability effects in ionic liquids. **C. Schröder**

Section E
Ernest N. Morial Convention Center
Room 223

Energy & Charge Transfer at Nanoscale Interfaces

Interfacial Charge Transfer in Emerging Mateirals

L. Huang, K.A. Willets, *Organizers*
S.T. Roberts, *Organizer, Presiding*
G. Schlau-Cohen, *Presiding*

8:30 PHYS 240. Probing coupled charge transfer and ion transport in nanostructured thin films. **D.S. Ginger**

9:00 PHYS 241. Charge and energy transfer in 2D colloidal semiconductor nanoplatelet quantum wells. B.T. Diroll, C.E. Rowland, I. Fedin, P. Darancet, A.O. Govorov, D.V. Talapin, **R.D. Schaller**

9:30 PHYS 242. Energy transfer dynamics and hot electron generation in Mn-doped $CsPbX_3$ nanocrystals. **D.H. Son**

9:50 PHYS 243. Evolution of defects at the lead halide perovskite/graphene oxide interfaces by *In situ* spectroscopy. **M. Acik**, I. Park, R.E. Koritala, G. Lee, R. Rosenberg

10:10 Intermission.

10:30 PHYS 244. Charge transfer excitons at van der Waals interfaces. **X. Zhu**

11:00 PHYS 245. Interfacial exciton dynamics in atomically thin semiconductors. **W.A. Tisdale**

11:30 PHYS 246. Highly mobile charge-transfer excitons in two-dimensional tetracene-WS_2 heterostructures. **T. Zhu**, L. Yuan, Y. Zhao, M. Zhou, Y. Wan, J. Mei, L. Huang

11:45 PHYS 247. Molecular photoelectronics at a rectifying gallium arsenide interface. **A. Vezzoli**, R. Brooke, N. Ferri, S.J. Higgins, W. Schwarzacher, R. Nichols

12:00 PHYS 248. Withdrawn

Section F
Ernest N. Morial Convention Center
Room 224

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Cosponsored by COMP‡
M.S. Gordon, A. Krylov, R. Lindh, T.L. Windus, *Organizers*
S.S. Leang, *Presiding*

8:30 PHYS 249. Aces4: Computational chemistry with the super instruction architecture. **B. Sanders**

9:10 PHYS 250. The Molecular Sciences Software Institute. **T. Crawford**, C. Clementi, R.J. Harrison, T.L. Head-Gordon, S. Jha, A. Krylov, V.S. Pande, T.L. Windus

9:50 Intermission.

10:10 PHYS 251. Analyzing new HPC system designs and code modernizations necessary to utilize them. **L. Carrington**

10:50 PHYS 252. Large-scale parallelization of vibronic coupling calculations. **J.F. Stanton**, S. Rabidoux, V. Eijkhout

11:30 PHYS 253. Application of ANI deep learned potentials to general computational chemistry problems. **J.S. Smith**, K.D. Ranasinghe, C. Devereux, O. Isayev, A.E. Roitberg

Section G
Ernest N. Morial Convention Center
Room 225

Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments

Gas-Phase Reactions

H. Cuppen, *Organizer*
D.E. Woon, *Organizer, Presiding*
S.J. Klippenstein, *Presiding*

8:30 PHYS 254. Withdrawn

9:05 PHYS 255. Nonadiabatic dynamics of silicon chemistry. **A.H. Chang**, R. Kaiser

9:40 PHYS 256. Reaction rates and mechanism for the reaction of electronically excited sulfur dioxide with alkanes. **J.A. Kroll**, V. Vaida

10:00 PHYS 257. Theoretical investigation of possible formation routes of interstellar SiS. **M. Rosi**, L. Mancini, N. Balucani, N. Faginas Lago, C. Ceccarelli, B. Le Floch, D. Skouteris, L. Podio, C. Codella, F. Fontani

10:20 Intermission.

10:40 PHYS 258. How to obtain accurate diabatic surfaces governing the dissociative recombination of astrophysical ions. **D. Talbi**, D. Kashinski, P. Hickman

11:15 PHYS 259. Computational study of the formation of prebiotic molecules in the interstellar medium through gas-phase reactions. **A. Largo**, P. Redondo, C. Barrientos, F. Siro Brigiano, Y. Jeanvoine, R. Spezia

11:50 PHYS 260. High accuracy thermochemistry and kinetics of the HCN/HNC system. **K. Lee**, M.C. McCarthy

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Dreyfus Prize Symposium

Theory & Computation

Sponsored by MPPG, Cosponsored by COMP‡, PHYS‡ and PRES

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Chemistry of Molecular Electronics

Monolayers: Tunneling & Function

Sponsored by COLL, Cosponsored by PHYS

Activation of Light (C1-C4) Hydrocarbons: Theory & Experiments
Sponsored by CATL, Cosponsored by ENFL, INOR and PHYS

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Enabling Fundamental Advances in Catalysis & Surface Science

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

PCET PhotoCatalysis with Inorganic Molecules & Materials
Sponsored by INOR, Cosponsored by PHYS

TUESDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Rooms 219/220

PHYS Awards Symposium

M.A. Duncan, *Organizer, Presiding*

1:30 PHYS 261. Award Address
(Peter Debye Award in Physical Chemistry Sponsored by DuPont). Multiphoton processes and their nanoscale control: Impact on energy and healthcare. **P.N. Prasad**

2:05 PHYS 262. Award Address
(ACS Award in Theoretical Chemistry Sponsored by the ACS Division of Physical Chemistry). Theoretical chemistry's role in providing sustainable energy. **E.A. Carter**

2:40 PHYS 263. Award Address
(Joel Henry Hildebrand Award in the Theoretical and Experimental Chemistry of Liquids Sponsored by the ExxonMobil Research and Engineering Company). Widom's formula and the utility of chemical modeling in the theory of solutions. **L.R. Pratt**

3:15 Intermission.

3:40 PHYS 264. Award Address
(Ahmed Zewail Award in Ultrafast Science and Technology Sponsored by the Ahmed Zewail Endowment Fund established by the Newport Corporation). Ultrafast protection of charge carriers–toward defect tolerant semiconductors. **X. Zhu**

4:15 PHYS 265. Award Address
(E. Bright Wilson Award in Spectroscopy Sponsored by the ACS Division of Physical Chemistry). Reversed interfacial fractionation of carbonate and bicarbonate evidenced by X-ray photoemission spectroscopy. **R.J. Saykally**

4:50 PHYS 266. Award Address
(Irving Langmuir Award in Chemical Physics Sponsored by the American Chemical Society and the ACS Division of Physical Chemistry). Probing graphene chemistry and electronic structure in two dimensions: A sub-nanometer view. G.W. Flynn, **J. Yardley**

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, INOR, PHYS‡, PMSE‡ and PRES‡

Young Chemists & Water
Sponsored by YCC, Cosponsored by PHYS

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Mechanisms

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Dreyfus Prize Symposium

Theory & Computation

Sponsored by MPPG, Cosponsored by COMP‡, PHYS‡ and PRES

Insights into Structure, Function, Dynamics & Evolution of Enzymatic Mechanisms from Computational Simulation
Sponsored by COMP, Cosponsored by CINF, MEDI and PHYS

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Enabling Fundamental Advances in Catalysis & Surface Science

Sponsored by CATL, Cosponsored by ENVR, INOR and PHYS

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

PCET PhotoCatalysis with Inorganic Molecules & Materials
Sponsored by INOR, Cosponsored by PHYS

TUESDAY EVENING

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
Sponsored by POLY, Cosponsored by PHYS and PMSE

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

PCET PhotoCatalysis with Inorganic Molecules & Materials
Sponsored by INOR, Cosponsored by PHYS

WEDNESDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory

Materials & Molecular Modelling

Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
P. Gori-Giorgi, *Presiding*

8:30 PHYS 267. Exact factorization of the N-electron wave function and its relation to density functional theory. **E. Gross**

‡*Cooperative Cosponsorship*

9:00 PHYS 268. Constrained searches in density functional and wavefunction theories. **A.J. Cohen**, P. Mori-Sanchez

9:30 PHYS 269. Electron densities (still) in search of Hamiltonians. **S.R. Atlas**

10:00 Intermission.

10:15 PHYS 270. Importance of theory in density functional theory. **K. Burke**

10:45 PHYS 271. Calculating the Levy constrained search for the exact functional of density functional theory. **P. Mori-Sanchez**, A.J. Cohen

11:15 PHYS 272. Describing discontinuity in exchange-correlation functional and strong correlation with fractional-spin correction. **N. Su**, C. Li, W. Yang

11:30 PHYS 273. Systematic improvement of approximations with smooth Coulomb potentials. **C.E. Gonzalez**, T. Verstraelen, P. Ayers, A. Savin

Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Advanced Techniques

P.H. Vaccaro, *Organizer*
M. Caricato, *Organizer, Presiding*

8:30 PHYS 274. Quantum dynamics of chiral molecules including electroweak parity violation: From high resolution spectroscopy towards fundamental symmetries and asymmetries. **M. Quack**

9:10 PHYS 275. Coherent population transfer in chiral molecules using tailored microwave pulses. **M. Schnell**

9:50 PHYS 276. Streamlining coupled cluster response theory for chiroptical properties. **T. Crawford**

10:10 PHYS 277. Generating chiral fields with achiral silicon nanowire dimers. **B.M. Reinhard**, X. Zhao

10:30 Intermission.

10:50 PHYS 278. Better, faster chiroptical anisotropy. **B.E. Kahr**, A.T. Martin, S.M. Nichols

11:30 PHYS 279. Selected computational studies of optical activity and electronic spectra. **J. Autschbach**

Section C
Ernest N. Morial Convention Center
Room 221

Understanding the Complexity of the Nano/Bio Interface with Experiments & Computations

Nanoparticle-Surface Structure & Dynamics

F. Geiger, *Organizer*
C.F. Landes, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 PHYS 280. Proteins on particles. **C.J. Murphy**

9:05 PHYS 281. Molecular dynamics study of human serum albumin protein corona in an inorganic nanoparticle. **D.C. Malaspina**, J. Faraudo

9:25 PHYS 282. Understanding the protein corona one molecule and one nanoparticle at a time. **S. Link**

9:55 Intermission.

10:10 PHYS 283. Influence of proteins on nanoparticle interaction with model biological membranes. **J.A. Pedersen**, E. Melby, C. Allen, I.U. Foreman-Ortiz, C.J. Murphy, R. Hernandez

10:40 PHYS 284. Computational study of interfacial forces driving aggregation of ultrasmall nanoparticles in biofluids. **S.A. Hassan**

11:00 PHYS 285. Thermodynamics study of absorption of blood proteins to carbon nanotubes and exosomes by molecular dynamics simulations. **M. Watanabe**, T. Rickel, Z. Green, J. Lozenski

11:20 PHYS 286. Air/water and mineral/water interfaces characterized by Ab initio molecular dynamics, and related prebiotic chemistry. **M.P. Gaigeot**

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Structure

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
K. Shimizu, *Presiding*

8:30 PHYS 287. Implications of liquid structure on the vibrational spectra of ionic liquids. **C. Burba**

8:50 PHYS 288. Thermal and neutron scattering studies on alkylammonium-based ionic liquids with plastic-crystalline phases. **O. Yamamuro**, M. Nirei, M. Kofu, M. Matsuki, T. Yamada, T. Madhusudan

9:25 PHYS 289. The Importance of Polarizability in the Solvation of Molecular Solutes in ionic liquids: OHD-RIKES measurements and molecular dynamics simulations on mixtures of CS_2 and ionic liquids. **E.L. Quitevis**, R.M. Lynden-Bell

10:00 PHYS 290. Spectroscopic and calorimetric analysis of multiple ionic liquid phase transitions in bulk and thin film systems. **J. Wrona**, S.K. Shaw

10:20 Intermission.

10:35 PHYS 291. Mesoscopic structural organization in triphilic, fluorinated, room temperature ionic liquids. **O. Russina**

11:10 PHYS 292. Liquid structure and self-assembly in ternary ionic liquid systems. H. Jiang, R. Atkin, **G. Warr**

11:45 PHYS 293. Elucidating the microscopic mechanics of attractive cation-cation interactions in hydroxyl-functionalized ionic liquids by isomer-selective vibrational spectroscopy of the N_2-tagged, gas phase $(M^+)_2NTf_2^-$ ternary complexes. **F. Menges**, **H. Zeng**, T. Niemann, A. Strate, R. Ludwig, M.A. Johnson

Section E
Ernest N. Morial Convention Center
Room 223

Energy & Charge Transfer at Nanoscale Interfaces

Achieving Energy & Charge Transfer with Plasmonic Systems

L. Huang, S.T. Roberts, K.A. Willets, *Organizers*
R.R. Frontiera, E. Grumstrup, *Presiding*

8:30 PHYS 294. Antenna-reactor complexes for plasmonic photocatalysis. **N.J. Halas**

9:00 PHYS 295. Femtosecond stimulated Raman microscopy of charge transfer on nanometer and micrometer length scales. **R.R. Frontiera**

9:30 PHYS 296. All-Metal optical power conversion via tunneling of plasmonic hot electrons. **M.T. Sheldon**, N. Hogan, S. Wu

9:50 PHYS 297. Strong coupling between surface plasmon polaritons and excitons for silver nanowires. G. Beane, B. Brown, **G.V. Hartland**

10:20 Intermission.

10:40 PHYS 298. Probing the optical responses in metallic, alloyed, and semiconductor nanostructures with fast electron spectroscopy. **D.J. Masiello**

11:10 PHYS 299. Spectro-electrochemical microscopy on single plasmonic nanostructures. **W. Chang**, B.S. Hoener, H. Zhang, T. Heiderscheit, S.R. Kirchner, A.S. De Silva Indrasekara, R. Baiyasi, Y. Cai, P.J. Nordlander, S. Link, C.F. Landes

11:25 PHYS 300. Plasmon rulers as optical transducers for nanoscale charge transfer. S. Lerch, **B.M. Reinhard**

11:45 PHYS 301. Observation of single molecule plasmon-driven electron transfer in isotopically edited 4,4′-bipyridine gold nanosphere oligomers. **E. Sprague-Klein**, M.O. McAnally, D. Zhdanov, A. Zrimsek, V.A. Apkarian, T. Seideman, G.C. Schatz, R.P. Van Duyne

Section F
Ernest N. Morial Convention Center
Room 224

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Cosponsored by COMP‡
M.S. Gordon, A. Krylov, R. Lindh, T.L. Windus, *Organizers*
J. Ivanic, *Presiding*

8:30 PHYS 302. Coupling advanced sampling and quantum simulation methods. **G.A. Galli**

9:10 PHYS 303. The embedded quantum ESPRESSO software package. **M. Pavanello**

9:50 PHYS 304. Parallel computing enables predictive on-the-fly photodynamics simulations. **T. Shiozaki**

10:30 Intermission.

10:50 PHYS 305. Software infrastructure for generating and analyzing large datasets in quantum chemistry. **C.D. Sherrill**, L.A. Burns, D.G. Smith

11:30 PHYS 306. Quantum chemistry on Intel Xeon Phi processors: Opportunities and challenges. **Z. Rinkevicius**

12:10 PHYS 307. Coupled-cluster methods in single precision. **P. Pokhilko**, A. Krylov, E. Epifanovsky

Section G
Ernest N. Morial Convention Center
Room 225

Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments

Surface Interactions/Grain Chemistry

D.E. Woon, *Organizer*
H. Cuppen, *Organizer, Presiding*
T. Lamberts, *Presiding*

8:30 PHYS 308. Off-lattice microscopic Monte Carlo kinetics models of interstellar and laboratory ices. **R.T. Garrod**

9:05 PHYS 309. A hybrid QM/MM approach to calculate binding energies of radical species on crystalline water ice . **W.C. Sameera**, B. Senevirathne, S. Andersson, G. Nyman

9:40 PHYS 310. Controversial determination of a key parameter to astrochemistry: Adsorption energy. **F. Pauzat**

10:00 PHYS 311. Simulations of energy dissipation and non-thermal desorption on amorphous solid water. **A. Fredon**, H. Cuppen

10:20 Intermission.

10:40 PHYS 312. Role of grain surfaces in astrochemical processes. **A. Rimola**, P. Ugliengo, C. Ceccarelli, **N. Balucani**, **M. Sodupe**

11:15 PHYS 313. Experimental studies on the surface reaction of hydrogen sulfide with deuterium atoms on amorphous solid water at 10 K. **Y. Oba**

11:50 PHYS 314. Reaction experiments on H exposure of solid methanol at low temperatures. **Y. Yarnall**, H. Hidaka, Y. Oba, T. Hama, A. Kouchi, N. Watanabe

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Kinetics

Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

Catalysis & Surface Science Science Applied to the Destruction of Threat Agents

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PCET PhotoCatalysis with Inorganic Molecules & Materials
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Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory

Excited States/Dynamics

Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
V.N. Staroverov, *Presiding*

1:30 PHYS 315. Stochastic adventures in density functional theory and beyond. **R.R. Baer**, E. Arnon, Y. Cytter, M. Fabian, B. Schpiro, V. Vlcek, E. Rabani, D. Neuhauser

2:00 PHYS 316. The correlation factor model: Generalizations and applications. **M. Ernzerhof**

2:30 PHYS 317. Fully non-local exchange-correlation functionals from the mathematical structure of the strong-coupling limit of DFT. **P. Gori-Giorgi**, S. Vuckovic

3:00 PHYS 318. Temperature and the strong-interaction limit of density functional theory. **A. Pribram-Jones**

3:15 Intermission.

3:30 PHYS 319. Electron density errors in approximate density functional calculations. **G.I. Csonka**, P. Mezei

4:00 PHYS 320. Orbital-dependent improvements to density-functional approximations: Application to highly charged molecular anions. **M.R. Pederson**, J. Batool

4:30 PHYS 321. Dispersion interactions from the exchange-hole dipole moment. **E.R. Johnson**

5:00 PHYS 322. Noncollinear spins in density functional theory: Ground state formulation, linear response, stability and single particle excited states. **G. Scalmani**, F. Egidi, X. Li, M.J. Frisch

5:15 PHYS 323. DFT functional calibration from highly-accurate energies and densities at different correlation regimes. **E. Matito**

5:30 PHYS 324. Density functional theory for spectroscopy and thermochemistry. **M. Biczysko**

Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Surfaces & Materials

M. Caricato, P.H. Vaccaro, *Organizers*
C. Merten, *Presiding*

1:30 PHYS 325. Exploring chiral space in molecules and materials. **B. Feringa**

2:10 PHYS 326. Helical molecules in flatland: Chiral recognition, spin-filtering and molecular machines. **K. Ernst**

2:50 PHYS 327. Chiral recognition among helical non-planar aromatic hydrocarbons on metal surfaces. **A. Mairena**, L. Zoppi, J. Seibel, M. Parschau, A. Tröster, K. Grenader, A. Terfort, K. Ernst

3:10 PHYS 328. Optical rotation of diatomic, helical chains as a model for periodic systems. **T.C. Balduf**, T. Aharon, M. Caricato

3:30 Intermission.

3:50 PHYS 329. Chirality in gold and silver nanoclusters. **C.M. Aikens**, N. Karimova

4:30 PHYS 330. Theoretical studies on structure-property relationships in helicene derivatives: Towards a rational design of systems with desired properties. **M. Srebro-Hooper**

Section C
Ernest N. Morial Convention Center
Room 221

Understanding the Complexity of the Nano/Bio Interface with Experiments & Computations

Nanoparticle-Surface Structure & Dynamics

F. Geiger, C.F. Landes, *Organizers*
C. Payne, *Presiding*

1:30 PHYS 331. Simulation-guided design of monolayer-protected nanoparticles. **R. Van Lehn**

2:00 PHYS 332. Investigating the interaction of amyloidogenic proteins with gold nanoparticles by means of atomistic simulations. **S. Corni**

2:20 PHYS 333. Structural analysis by enhanced Raman scattering: Application to lipid membrane structures. **J.H. Hafner**, S. Demers, C. Shirazinejad, G. Isakson, J. Matthews

2:50 Intermission.

3:05 PHYS 334. Surface functionalization and ligand-receptor binding of Au nanorods: Effects of local curvature, polymer chemistry, and polymer architecture. **E. Gonzalez Solveyra**, D.C. Malaspina, I. Szleifer

3:25 PHYS 335. The molecular mechanism of nanodroplet stability. E. Zdrali, Y. Chen, H. Okur, D. Wilkins, **S. Roke**

3:55 PHYS 336. Altering protein crystallization by modulating salt concentration. **M. Olvera De La Cruz**

4:25 PHYS 337. DNA-templated fluorescent gold nanocluster-graphene composite: A multifunctional platform. **K. Perry**, R. Jimenez, S.P. Karna

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Transport & Dynamics

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
O. Russina, *Presiding*

1:30 PHYS 338. Simulations of friction on solute motion in ionic liquids. B. Conway, C.A. Rumble, **M. Maroncelli**

2:05 PHYS 339. Ionic liquid mobility on different time scales as seen from polar, apolar and solute perspectives. **C.J. Margulis**, R.P. Daly, J.C. Araque

2:25 PHYS 340. Influence of mesoscopic confinement on the dynamics of room temperature ionic liquids. **M.D. Fayer**

3:00 PHYS 341. Hydrogen bond dynamics in protic ionic liquids: Ultrafast vibrational spectroscopy of SCN-. **S. Garrett-Roe**

3:35 Intermission.

3:50 PHYS 342. Effects of mesoscopic domain structure on shear viscosity of ionic liquids. **T. Yamaguchi**

4:25 PHYS 343. Molecular origin of enhanced proton conductivity in anhydrous ionic glasses. **Z. Wojnarowska**, L. Tajber, J. Knapik-Kowalczuk, M. Paluch

4:45 PHYS 344. Influence of mesoscale organization on charge transport and dynamics in ionic liquids. **T. Cosby**, Z. Vicars, M. Heres, K. Tsunashima, J. Sangoro

Section E
Ernest N. Morial Convention Center
Room 223

Energy & Charge Transfer at Nanoscale Interfaces

Using Quantum Dots to Direct Charge & Energy Transfer

L. Huang, S.T. Roberts, K.A. Willets, *Organizers*
L. Nienhaus, J. Vura-Weis, *Presiding*

1:30 PHYS 345. Interfacial charge transfer as a probe of the electrostatic potential of a colloidal quantum dot. C. He, **E.A. Weiss**

2:00 PHYS 346. Excited state dynamics at nanoscale interfaces for solar energy harvesting: Time-domain Ab initio studies. **O.V. Prezhdo**

2:30 PHYS 347. Improving energy migration in nanocrystal solids ligand exchanged with exciton-delocalizing ligands. **M.S. Azzaro**, A. Dodin, D.Y. Zhang, A.P. Willard, S.T. Roberts

2:45 PHYS 348. Interfacial control of colloidal heteronanostructures to control single particle emission in Cd-based and CuIn-based chalcogenide quantum dots. **C.D. Heyes**

3:05 Intermission.

3:25 PHYS 349. Directing triplets across the nanocrystal-molecule interface. **M.L. Tang**, Z. Huang, P. Xia, E. Moses

3:55 PHYS 350. Colloidal semiconductor nanocrystal photocatalysts: Teaching an old dot new tricks. C. Liu, F. Qiu, L. Frenette, R. Burke, **T.D. Krauss**

4:25 PHYS 351. Charge-trapping at the surfaces of nanocrystals vs charge-transfer on the nanoscale. **P. Kambhampati**

4:45 PHYS 352. Biexciton and trion energy transfer from CdSe/CdS giant nanocrystals to Si substrates. T. Guo, S. Sampat, S.M. Rupich, J.A. Hollingsworth, M. Buck, H. Htoon, Y.J. Chabal, Y. Gartstein, **A. Malko**

5:05 PHYS 353. Photoreductive dissolution of cerium oxide nanoparticles upon UV irradiation. **N.W. Pettinger**, S. Froebel, J. Empey, S. Natarajan, B. Wynne, B. Kohler

Section F
Ernest N. Morial Convention Center
Room 224

Quantum Chemical Program Development in a Modern Computer & Programming Environment
Cosponsored by COMP
M.S. Gordon, A. Krylov, R. Lindh, T.L. Windus, *Organizers*
B. Sanders, *Presiding*

1:30 PHYS 354. *LibEFP* as a route to a general explicit and implicit solvent functionality. **L.V. Slipchenko**

2:10 PHYS 355. Enhancing scalability of the effective fragment molecular orbital method: OpenMP parallelization for MAKEFP. **A. Gunina**, M.S. Gordon

2:50 Intermission.

3:10 PHYS 356. Exploiting graphical processing units to enable accurate excited state potential energy surface calculation for large molecules. **F. Liu**, M. Filatov, T.J. Martinez

3:50 PHYS 357. A comprehensive assessment of accuracies and system scaling properties of electron correlation procedures, leading to a new hybrid correlation energy (HyCE) approach. **J. Ivanic**, M.W. Schmidt

4:30 PHYS 358. Multilevel many-body expansion for fragment-based methods. **B. Westheimer**, M.S. Gordon

Section G
Ernest N. Morial Convention Center
Room 225

Quantum Chemistry, Dynamics & Reaction Modeling for Molecules & Materials in Astrophysical Environments

Grain Chemistry / Modeling: Protostellar Disks

D.E. Woon, *Organizer*
H. Cuppen, *Organizer, Presiding*
R.T. Garrod, *Presiding*

1:30 PHYS 359. Reactivity of atoms and molecules on interstellar ice analogs at low temperatures. **T. Lamberts**, J. Kästner

2:05 PHYS 360. Methanol-containing ice mantle on collision with $OH^{\cdot}$: A dust grain reaction through quantum *ab initio* molecular dynamic. **N. Inostroza**

2:40 PHYS 361. Mechanisms of SiO oxidation: Implications for dust formation. **S. Andersson**

3:00 PHYS 362. Trapping of molecular oxygen in cometary ices: solid state modeling. **A. Markovits**

3:20 Intermission.

3:40 PHYS 363. New constraints on the chemistry of planet formation. **E. Bergin**

4:15 PHYS 364. Gaining insights into protoplanetary disk conditions from chemistry. **U. Gorti**

Unconventional Catalysis Targeting Stable Molecules

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Catalytic & Photocatalytic Degradation of Pollutants & Chemical Threat Agents: New Developments in Materials & in In-situ & Operando Methods

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PCET PhotoCatalysis with Inorganic Molecules & Materials
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WEDNESDAY EVENING

Section A
Ernest N. Morial Convention Center
Hall D

PHYS Poster Session

M.A. Duncan, *Organizer*

7:00–9:00

PHYS 365. Quantum control for chemical reaction of particles at surface. **Q. Wang**

PHYS 366. Direct visualization of hot-carrier transport in hybrid perovskites to overcome the Shockley-Queisser limit. **J. Snaider**, L. Huang

PHYS 367. Withdrawn

PHYS 368. Hydrogen permeation properties of a Pd-based metallic glass. **X. Du**

PHYS 369. The Closo-$Si_{12}C_{12}$ molecule from cluster to crystal: Design charge transfer excitonics polymers with siloxane and silane links. **X.F. Duan**, L. Burggraf

PHYS 370. Energy dependent electron transfer dynamics at dye-bridge-semiconductor interface. **J.C. Wang**, K. Violette, M. Sykora, K. Hanson

PHYS 371. Heterodyne-detected vibrational sum frequency generation spectroscopy for buried electrode/electrolyte solution interfaces. **S. Nihonyanagi**, A. Sayama, Y. Ohshima, T. Tahara

PHYS 372. Measurements and analysis of ultrafast transient absorption spectra of YOYO-1 in solutions. **J. Chen**, L. Wang, J.R. Pyle

PHYS 373. Enhanced thermoelectric properties in graphene/bismuth telluride/graphene (Gr/Bi_2Te_3/Gr) heterostructures. **D.S. Choi**, K. Perry, **S.P. Karna**

PHYS 374. Scaling tensor contractions in the post Moore's law computing era. **K. Ibrahim**

PHYS 375. Withdrawn

PHYS 376. Withdrawn

PHYS 377. Excited state dynamics of charge carriers at the interfaces: Insights from nonadiabatic molecular dynamics calculations. **A. Nijamudheen**, A.V. Akimov

PHYS 378. Withdrawn

PHYS 379. Using Fano resonances to measure and control photonic-plasmonic hybridization. **K.C. Smith**, D.J. Masiello

PHYS 380. Solvent effect and tunneling corrections on the intermolecular proton transfer of the guanine-cytosine and adenine-thymine DNA base pairs: A polarizable continuum model study. **E. Romero**, F. Hernandez

PHYS 381. Large-scale first principles NMR calculations with numeric atom-centered basis sets. **R. Laasner**, W. Huhn, J. Colell, T. Theis, W.S. Warren, V.W. Yu, V. Blum

PHYS 382. GPU-accelerated large-scale electronic structure theory with a first-principles all-electron code. **W.P. Huhn**, B. Lange, V. Yu, S. Lee, M. Yoon, V. Blum

PHYS 383. Withdrawn

PHYS 384. Plasmon enhanced electrochemical dissolution of gold nanorods. **B. Hoener**, S.S. Collins, S.R. Kirchner, W. Wang, S.H. Jebeli, A. Joplin, W. Chang, S. Link, C.F. Landes

PHYS 385. Structural factor in radical enhanced intersystem crossing of BODIPY. **Y. Cao**, Y. Huang, Z. Xu, T. Jin, T. Lian, E. Egap

PHYS 386. Information entropies in single molecule studies. **M.A. Ochoa**

PHYS 387. Probing the (110)-oriented plane of rutile ZnF_2: A DFT investigation. **A. Abbaspour Tamijani**

PHYS 388. Accelerating excited state molecular dynamics using an extended Lagrangian. **J. Bjorgaard**, D. Sheppard, S. Tretiak, A. Niklasson

PHYS 389. Influence of size of nanoparticles on their XRD patterns: Insights from modeling. **A.V. Vorontsov**

PHYS 390. Layered tetragonal zinc chalcogenides for energy-related applications: From photocatalysts for water splitting to cathode materials for Li-Ion batteries. **J. Zhou**

PHYS 391. Photo-carrier generation and separation in two-dimensional vertical and lateral heterostructures. **L. Yuan**, L. Huang

PHYS 392. Exploring the relationship between plasmon damping and luminescence QY in lithographically prepared gold nanorods. **L.J. Tauzin**, Y. Cai, K.W. Smith, W. Chang, C.F. Landes, S. Link

PHYS 393. Charge transfer through surface and bulk midgap states in titanium dioxide and metal titanates: Exciton and water as probes in novel synchronous versus "conventional" luminescence spectroscopy. **A. Samokhvalov**, S. Taylor

PHYS 394. Photoluminescence of gold nanorods: Purcell effect enhanced emission from hot carriers. **Y. Cai**, J.G. Liu, L.J. Tauzin, D. Huang, E.R. Sung, H. Zhang, A. Joplin, C.F. Landes, W. Chang, P.J. Nordlander, S. Link

PHYS 395. Probing structural rearrangements during rubrene singlet fission using femtosecond stimulated Raman spectroscopy. **K. Bera**, C.J. Douglas, R.R. Frontiera

PHYS 396. Measuring buried interfacial electronic structure using heterodyne detected electronic sum frequency generation. **A.P. Moon**, J.A. Bender, D.E. Cotton, B.A. Renard, S.T. Roberts

PHYS 397. Directional response from disorder: Exploiting the interplay between nanoscale disorder and non-equilibrium exciton and charge transport. **A. Dodin**, A.P. Willard

PHYS 398. Damping of acoustic vibrations in gold nanowires. **T. Devkota**, K. Yu, G.A. Beane, G.V. Hartland

PHYS 399. Refined potential for LiTFSI-Acetonitrile electrolyte system. **Z. Li**, L. Robertson, I.A. Shkrob, Y. Cao, L. Zhang, J. Moore, Y. Zhang

PHYS 400. Understanding charge transfer from metal oxide nanocrystals to organic semiconductors following LSPR excitation. **M. Blemker**

PHYS 401. Structure-based exciton Hamiltonian and dynamics for the reconstituted wild type CP29 protein antenna complex of the photosystem II. **M. Jassas**, J. Chen, A. Khmelnitskiy, A.P. Casazza, S. Santabarbara, R. Jankowiak

PHYS 402. Plasmon damping at the nanoparticle surface. **B. Foerster**, A. Hoggard, K. Kaefer, S. Celiksoy, W. Chang, S. Link, C. Sönnichsen

PHYS 403. Modifying the hybridization of transition metal *d* orbitals with weak external fields. **P. Darapaneni**, A.M. Meyer, K. Lopata, O. Kizilkaya, J.A. Dorman

PHYS 404. Low temperature high resolution spectroscopic and modeling studies of the wild type and mutant FMO antenna from *C. tepidum*. **A. Khmelnitskiy**, R. Saer, R.E. Blankenship, R. Jankowiak

PHYS 405. Computational mechanistic insights into the palladium-catalyzed alkylation of selected aldehyde-derived hydrazones. A.D. Bani-Yaseen, **E. Elbashier**, F. ElNamla, N. Odeh

PHYS 406. Quantum framework to resonant energy transfer under the influence of the metal surface evanescent field. **X. Chen**, A. Poudel, M.A. Ratner

PHYS 407. Comparison of the barrier properties of PVD and ALD deposited Ta based materials for Cu diffusion. **K. Muthukumar**, A. Basu, B. Sheu, L. Chen, Z. Wu, R. Shaviv, J.J. Lee, T. Hong Ha, X. Tang

PHYS 408. Advances in rational design of modified proton reduction catalysts. **M. Davis**, C.N. Virca, T. McCormick

PHYS 409. Ultraviolet absorption spectra of charge transfer to solvent transitions for aqueous halide and hydroxide ions in subcritical water. **T.W. Marin**, **I. Janik**

PHYS 410. Dynamic stabilization of metal oxide / liquid water interfaces through water exchange. **G. von Rudorff**, M. McBriarty, J. Stubbs, P.J. Eng, J. Blumberger, K. Rosso

PHYS 411. Structure and dynamics of the hematite(001)-liquid water interface: pKa estimates from thermodynamic integration and hydrogen bond patterns. **G. von Rudorff**, R. Jakobsen, O. Gittus, K. Rosso, J. Blumberger

PHYS 412. Accelerating hybrid functional-based molecular dynamics simulation through screening of Hartree-Fock exchange forces. **G. von Rudorff**, R. Jakobsen, K. Rosso, J. Blumberger

PHYS 413. A mixed resolution protocol to assess ionic liquid effects on biological system. **A.J. Heyert**, G.E. Lindberg

PHYS 414. ELSI: A unified software interface for Kohn-Sham electronic structure solvers. **V. Yu**, W.P. Huhn, L. Lin, J. Lu, A. Vazquez-Mayagoitia, C. Yang, V. Blum

PHYS 415. Competitive adsorption of environmentally relevant anions on lithium ion battery cathode materials. **D. Jones**, J.W. Bennett, A. Abbaspour Tamijani, S.E. Mason

PHYS 416. Selenium NMR spectroscopy: A versatile probe for biological macromolecules. **S. Rozovsky**

PHYS 417. Untangling the details of surfactant assembly at the nanoemulsion interface. **A. Carpenter**, R. Altman, R. Ciszewski, G.L. Richmond

PHYS 418. Energy and mass transfer analysis of foam fluid in porous media. **S. Liu**

PHYS 419. Withdrawn

PHYS 420. Self-organization of layered inorganic membranes in microfluidic devices. **Q. Wang**, M.R. Bentley, O. Steinbock

PHYS 421. Acoustic interactions of biochar with CO_2 and H_2O: Experimental and theoretical approaches. **T. Zubatiuk**, B. Sajjadi, G.A. Hill, D. Leszczynska, W.W. Chen, J.R. Leszczynski

PHYS 422. Ab Initio calculations of possible heptacoordinate and octacoordinated carbon in ionic hydrocarbon compounds. G. Wang, **A. Rahman**, B. Wang

PHYS 423. Modeling electrolyte mixtures with concentration dependent dielectric permittivity. **H. Chen**, A. Panagiotopoulos

PHYS 424. Psi4NumPy: An interactive quantum chemistry programming environment. D.G. Smith, L.A. Burns, **D. Sirianni**, D.R. Nascimento, A. Kumar, A. James, J.B. Schriber, T. Zhang, B. Zhang, A. Abbott, E. Berquist, M. Lechner, L. dos Anjos Cunha, A.C. Simmonett, J. Turney, F.A. Evangelista, A.E. DePrince, T. Crawford, K. Patkowski, C.D. Sherrill

PHYS 425. Gas phase studies of ionic liquids. **E.L. Collins**, G. Liu, S. Marquez, S. Ciborowski, M. Marshall, Z. Zhu, J. Damewood, A. Buytendyk, J. Graham, K.H. Bowen

PHYS 426. Withdrawn

PHYS 427. Phase transitions and chemical instability of an ionic liquid under high pressure. **L.F. Faria**, M. Medre, R. Bini, M.C. Ribeiro

PHYS 428. Small polaron in zero-dimensional perovskite Cs_4PbBr_6. **J. Yin**, P. Maity, M. De Bastiani, I. Dursun, O.M. Bakr, J.E. Bredas, O.F. Mohammed

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PHYS 429. Solvent-ion structure and thermodynamics of a nitromethane-tetrahydrofuran lithium ion cluster. E. Curotto, **D. Bierwisch**, A. Fodor, M.J. Hyers

PHYS 430. Response of differently doped semiconductors to light with orbital angular momentum. **P. Navotnaya**, B. Rolczynski, G.S. Engel

PHYS 431. Tuning the photochemical reactivity of electrocyclic reactions using substituents–a non-adiabatic molecular dynamics study. **T.W. Thompson**, E. Tapavicza

PHYS 432. Fluorescence lifetime studies of calmodulin-eNOS complexes. **K. Guadalupe**, S. Bailey, C.K. Johnson

PHYS 433. Experimental and theoretical investigations of infrared multiple photon dissocation spectra of lysine complexes with Zn^{2+} and Cd^{2+}. **C. Owen**, G. Boles, G. Berden, J. Oomens, P. Armentrout

PHYS 434. pH dependent interaction of norfloxacin housed in lysozyme: The protein modulates the prototropic equilibrium of the drug to host the preferred ionized state. **I. Das**, M. Halder

PHYS 435. Withdrawn

PHYS 436. Absorbance and fluorescence spectra of 5-(benzylidene) pyrimidine-2,4,6-triones. **N. Barashkov**, **T. Sakhno**, A. Mantel, A. Aldongarov, D. Birimzhanova, I. Irgibayeva

PHYS 437. Theoretical studies of cytochrome c peroxidase–cytochrome c electron transfer: The role of tryptophan. **X. Ru**, P. Zhang, D.N. Beratan

PHYS 438. Photochemical study of Coenzyme B_{12}-dependent enzymes: Theoretical study. **A. Mamun**, P.M. Kozlowski

PHYS 439. Mechanism of Alkyl transfer reaction involving Cob(I)Alamin by Alkyl halide: S_N2 or radical mechanism? **A. Ghosh**, P.M. Kozlowski

PHYS 440. Molecular dynamics studies of ordering of ionic liquids at interfaces. **W.D. Amith**, J.J. Hettige, **W.V. Karunaratne**, E. Castner, C.J. Margulis

PHYS 441. Classical, semi-empirical and first principles dynamic of excess charges in ionic liquids. **F. Wu**, C. Xu, C.J. Margulis

PHYS 442. Modeling quantum effects on metabolism rate in deuterated drugs. **C.P. Schultz**, J.W. Mazzuca

PHYS 443. Infrared spectroscopic investigation of carbonyl sulfide hydration in superfluid helium nanodroplets. **T.W. Faulkner**, I. Miller, P. Raston

PHYS 444. Super atomic nature of $Be(NH_3)_4$. **I. Ariyarathna**, S. Khan, E. Miliordos

PHYS 445. Quantum chemical strategies for determining properties and reaction behavior for astrochemical applications. **D.E. Woon**

PHYS 446. New computational methodology for modeling sum frequency spectra of large molecules. **R. Altman**, N.A. Valley, G.L. Richmond

PHYS 447. Real time studies of triglyceride thermal cracking chemistry using molecular beams. **I. Alhroob**, E. Kozliak, **A. Kubatova**, **M. Sulkes**

PHYS 448. Multiconfiguration pair-density functional theory: Theory and applications to spin-multiplicity splitting, transition metal bond energies, and the abyss of delocalization error. **J.L. Bao**, D.G. Truhlar, L. Gagliardi

PHYS 449. Ab-initio calculations on the ground and excited electronic states of palladium monoxides, $PdO^{0,+,-}$. **N. Almeida**

PHYS 450. Acrylic and propiolic sulfuric anhydrides: Formation, microwave characterization, and theoretical calculations. **C.J. Smith**, A. Huff, R.B. Mackenzie, K.R. Leopold

PHYS 451. Proton-coupled electron transfer and substituent effects in catechol-based deep eutectic solvents: Gross and fine tuning of redox activity. **P.J. Smith**, J.C. Goeltz

PHYS 452. Phase transitions of ionic liquids in nanoconfinement. **F. Sorourifar**, G. Jeanmairet, M. Salanne, B. Rotenberg, B. Coasne

PHYS 453. Theoretical investigation of monomers self-assembly through hydrogen-bonding and π-stacking. **M. Boraghi**, J. I-Chia Wu

PHYS 454. Internal rotation and monohydration of carboxylic sulfuric anhydrides. **A.K. Huff**, C.J. Smith, R.B. Mackenzie, K.R. Leopold

PHYS 455. In-situ second-harmonic generation of gold nanoparticle growth and ultrafast reflectivity on $La_{0.67}Sr_{0.33}MnO_3/SrTiO_3$. **R. Khoury**, J.C. Ranasinghe, J. Taylor, M. Saghayezhian, A.S. Dikkumbura, W. Plummer, L.H. Haber

PHYS 456. Role of the first excited state of atomic oxygen (^1D) in the formation of "hypervalent" iodine-oxygen compounds and the oxidation mechanism of alkenes by such species. **N. Khan**

PHYS 457. Linking pH, temperature, K^+ concentration and conformation for the DNA i-motif. C.R. Fraire, T. Nguyen, S. Sullivan, S. Tittle, E. Bazan, **R.D. Sheardy**

PHYS 458. Ultrafast excited state transport and decay dynamics in cesium lead mixed-halide perovskites. **C.L. Kennedy**, A. Hill, E.S. Massaro, E. Grumstrup

PHYS 459. Alkyne combustion: Experimental and theoretical studies of formyl radical formation. **M. Drummer**, R.W. Quandt, J.M. Standard

PHYS 460. Modeling proton transfer of 5-amino-2-naphthol and 8-amino-2-naphthol. **K. Nelson**, M. Groves, L. Cotter, K. Takematsu

PHYS 461. Entangeled trajectory Hamiltonian dynamics. **B. Smith**, A.V. Akimov

PHYS 462. Characterizing the effect of particle size on deposition in printed human models. J. Kesavan, **V. Alstadt**, J.R. Bottiger, B.L. Laube

PHYS 463. Reduction of CO_2 and N_2 using the Li_3F_2 superalkali. **H. Park**, G. Meloni

PHYS 464. Synchrotron photoionization study of furan and 2-methylfuran reactions with methylidyne radical (CH) at 298 K. **E. Carrasco**, G. Meloni, K. Smith

PHYS 465. Analytic gradient for the effective fragment molecular orbital (EFMO) charge transfer energy. **S. Kim**, P. Xu, C. Bertoni, M.S. Gordon

PHYS 466. Simulations and spectroscopy of interfacial environments in lipid membranes. **M. Valentine**, C.R. Baiz

PHYS 467. Comparison of theoretical and experimental electron density distributions of 1-methyl-4-imidazoline-2-thione. **S. Hornback**, S. Khan, **E.D. Stevens**

PHYS 468. Ultrafast radiationless relaxation dynamics of low-energy near-infrared excited electronic states of Cu(II) and Ir(IV) complexes. **D. Budkina**, S.M. Matveev, C.M. Hicks, V.A. Borin, A.S. Mereshchenko, A.N. Tarnovsky

PHYS 469. Astrobiological explorations of amino-substituted nucleobase anions. **A.A. Dobbs**, D.T. Novoa, A.R. Wegener, C. Cole

PHYS 470. Long-lived complexes and quantum chaos in ultracold collisions. **J.F. Croft**, B. Naduvalath, B. Kendrick

PHYS 471. Applications of two-dimensional white-light spectroscopy utilizing conjugated aromatic systems. **N.R. Fetto**, M.J. Tucker

PHYS 472. Development of a coarse-grained model of polypeptoids for studying self-assembly in solution. **P. Du**, R. Kumar

PHYS 473. A quantitative and spatially-resolved accounting of the performance-bottleneck in high efficiency, planar hybrid perovskite solar cells. **S. Draguta**, J. Christians, J. Luther, M.K. Kuno

PHYS 474. Theoretical investigation of cyanopolyynes as the coloring agents of Jupiter's Great Red Spot. **C. Davis**, M. Dorko

PHYS 475. High-accuracy electronic structure calculations of the acetylperoxy/HO_2 reaction mechanism. **K.T. Kuwata**, M.P. DeVault

PHYS 476. Proton transfer in 7-amino-2-naphthol. **L. Cotter**, R. Nelson, K. Takematsu

PHYS 477. Model chemistries for ground and excited states: Long-range corrected hybrid density functional theory. **J.L. Sonnenberg**, G. Scalmani, G.W. Trucks, M.J. Frisch, K.B. Wiberg

PHYS 478. Observation of ultrafast vibrational energy transfer. **M. Ashner**, W.A. Tisdale

PHYS 479. Molecular adsorption and resonance coupling at the colloidal silver–gold core–shell nanoparticle interface. **A.S. Dikkumbura**, H.T. Smith, R.A. Khoury, J.C. Ranasinghe, L.H. Haber

PHYS 480. Ultrafast transient absorption spectroscopy of porphyrin based NanoGUMBOS, silver-gold core-shell and silicon nanoparticles. **J.C. Ranasinghe**, T.E. Karam, A.S. Dikkumbura, R.A. Khoury, N. Siraj, I.M. Warner, L.H. Haber

PHYS 481. Cation effect on the solvent structure of trifluoroacetamide based deep eutectic solvents. **Y. Cui**, D.G. Kuroda

PHYS 482. Acetate ion and its interesting solvation shell. **X. Zhang**, D.G. Kuroda

PHYS 483. Structure and dynamics of ion pairs in glymes. **S. Galle Kankanamge**, D.G. Kuroda

PHYS 484. Investigation of structure and dynamics of glyme based electrolytes for sodium rechargeable batteries. **K. Li**, S. Galle Kankanamge, P. Du, R. Jorn, R. Kumar, D.G. Kuroda

PHYS 485. Sodium binding interactions with the aliphatic amino acids: A guided ion beam and computational study. **H. Pham**

PHYS 486. Fragmentation of deprotonated n-methylguanine anions. **D. Novoa**, A. Wegener, A.A. Dobbs, C. Cole

PHYS 487. Separation of chiral molecules by enantio-specific interactions using magnetic surfaces. **E. Capua**, K. Banerjee-Ghosh, F. Tassinari, O. Ben Dor, S. Yochelis, Y. Paltiel, R. Naaman

PHYS 488. Microscopic dynamics and thermal properties of glycine betaine solutions. **N. Yamamuro**, N. Murase, M. Kofu, T. Kikuchi, O. Yamamuro

PHYS 489. Air/water and silica/water interfaces characterized by Ab Initio Molecular Dynamics. **S. Pezzotti**, D. Galimberti, F. Siro Brigiano, M.P. Gaigeot

PHYS 490. Hulburt-Hirschfelder potential for the ground state of Li_2, Na_2, and K_2. **L. Biolsi**

PHYS 491. Photophysics and charge localization of azothiazol-dithiophene conjugated polymers. **A. Alsam**, O. Mohammed, N. Hadjichristidis

PHYS 492. Spin-controlled electrochemistry using chiral electrodes: Effects on water electrolysis. **F. Tassinari**, W. Mtangi, K. Banerjee-Ghosh, B. Adelizzi, F. Parenti, K. Vankayala, A. Palmans, A. Vargas Jentzsch, C. Fontanesi, A. Mucci, E.W. Meijer, R. Naaman

PHYS 493. Withdrawn

PHYS 494. Visualizing the dimensionality-dependent evolution of a semiconductor's electronic structure. M.P. McDonald, **R. Chatterjee**, J. Si, B. Jankó, M.K. Kuno

PHYS 495. Effect of small perturbations on the Belousov-Zhabotinsky reaction. **M.S. Zahed**, H.M. Hastings

PHYS 496. Stabilizing effects in carboraneselenolate self-assembled monolayers. **D.P. Goronzy**, J. Thomas, A.M. Spokoyny, C.A. Mirkin, P.S. Weiss

PHYS 497. Spectroscopic study of a C_4H_5 radical: 2-butyn-1-yl. **M. Ellis**, G. Brown, O. Bhatti, L.R. McCunn

PHYS 498. Vibrational spectroscopy of a

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substituted propargyl radical: 1-butyn-3-yl. **G. Brown**, M. Ellis, O. Bhatti, L.R. McCunn

PHYS 499. Photochemistry of dipyridinylphenanthrenedioxin-copper complexes. **K. Karabaeva**, D. Budkina, R.M. Wilson, A.N. Tarnovsky, L. Sallans

PHYS 500. Computational investigations of the graphene oxide – liquid interface. **V. Subasinghege Don**, P. Du, R. Kumar

PHYS 501. High-resolution infrared spectroscopy of SC_3S and SC_2S carbon-sulfur clusters. **J.B. Dudek**, S.K. Bentley, T. Salomon, S. Fanghänel, S. Thorwirth

PHYS 502. Chitosan assisted synthesis of silver hexahedrons on disposable pencil graphite electrode: Low–cost sensor for hydrogen peroxide and hydrazine. **P. Sankaranarayanan**, S.M.V.

PHYS 503. Poking surfaces: Absolute, interferometric, complex spectral measurement. **M.J. Shultz**, P.J. Bisson, J.M. Marmolejos, J. Wang

PHYS 504. Understanding material characteristics through fingerprint traits from helium pycnometry. **H.T. Nguyen**, J. Horn, M. Bleakney, S. Hudson, L. Espinal

PHYS 505. Size and solid concentration effects in surface complexation models. **J. Luetzenkirchen**, T. Klacic, T. Preocanin

PHYS 506. Characterization of monovalent and divalent ion interactions in interfacial esters. **E. Ma**

PHYS 507. Femtosecond time-gated absorption spectroscopy (fs-TGAS): Development of a robust method for measuring broadband, background-free absorption spectra. **P.S. Walsh**, H.U. Stauffer, S. Roy, J.R. Gord

PHYS 508. Flying into the future of heat management on the wings of chemical reactions. **A. Widstrom**, A. Katona, B.J. Lear

PHYS 509. Effect of adding sodium chloride on the thermodynamic characterizations of tetra-n-butylammonium chloride/water semi-clathrate system. **M. Siddiq**

PHYS 510. Detailed kinetic modeling of biochemical pathways using PySB. **Z. Kamdar**, **R.J. Olsen**, E.C. Pollock

PHYS 511. Ultrafast time-resolved dynamics of singlet fission in diphenylisobenzofuran derivative on film. **M.A. Hermosilla**, V.D. Kleiman, K. Hanson, S.P. Hill, T. Banerjee

PHYS 512. Conformational changes in alpha-synuclein in the presence of aqueous ionic liquids probed with FRET measurements. **B.L. Stinger**, T.D. Vaden

PHYS 513. Analysis of carboplatin and DNA interactions by spectroscopic techniques. **C.R. Fraire**, S.M. Williams, R.D. Sheardy, N. Mirsaleh-Kohan

PHYS 514. Ion transport properties in mixed ionic liquid/carbonate electrolytes for Li-ion batteries. **M. Ebrahiminia**, K. Oldiges, D. Diddens, D. Bedrov

PHYS 515. Strong parallel scaling for sparsity-screened density-fitted integrals on Knights Landing. **M.C. Schieber**, D.G. Smith, E. Chow, C.D. Sherrill

PHYS 516. Ion dynamics in doubly-charged DABCO-containing copolymers of n-butyl acrylate. **M. Harris**, K. Drummey, T.E. Long, J. Sangoro

PHYS 517. Three-body hydrogen bond defects contribute significantly to the dielectric properties of the liquid water-vapor interface. **S. Shin**, A.P. Willard

PHYS 518. Femtosecond extreme ultraviolet transient absorption spectroscopy explorations of bromobenzene. **L. Heald**, S. Sutton, S.G. Sayres

PHYS 519. Understanding how cisplatin and carboplatin modify DNA bases. **T. Nguyen**, S. Wappes, N. Mirsaleh-Kohan

PHYS 520. Kinetic studies of molecular scale heating using the photothermal effect. **E. Van Burns**, B.J. Lear

PHYS 521. Optimizing triplet exciton transfer from lead calcogenide nanocrystals to TIPS-Pentacene ligands for photon upconversion. **E.K. Raulerson**, **J.A. Bender**, X. Li, M.L. Tang, S.T. Roberts

PHYS 522. Solvent-dependence of the phenol-benzene H-π equilibrium constant. **K.J. Feierabend**, B.B. Bowers

PHYS 523. Exploring the structural effects of nedaplatin and carboplatin on a short DNA oligonucleotide. **M. Garrett**, **A. Lanka**, S. Ariyibi, N. Mirsaleh-Kohan

PHYS 524. Energy of the quasi-free electron in CO and HD: Extension of the local Wigner-Seitz model to polar fluids. **C.M. Evans**, J. Hare, G.L. Findley

PHYS 525. Energy of the quasi-free electron in supercritical and near critical CF_4. **J. Hare**, B. Flor, C.M. Evans, G.L. Findley

PHYS 526. Investigating the mechanism of water loss in cationic clusters containing dicarboxylic acids. **K.A. Nickson**, S.E. Waller, C.J. Johnson

PHYS 527. A spectroscopic and theoretical study of dipole-bound anions of indazole derivatives. **A. Williams**, N. Hammer

PHYS 528. Identifying key charge migration modes with time-depdendent density functional theory. **A. Bruner**, S. Hernandez, F. Mauger, P. Abanador, M. Gaarde, K. Schafer, K. Lopata

PHYS 529.
Experimental and theoretical investigation of the phase stability of methane and ethane mixtures at temperatures relevant to the outer solar system. **S. Dustrud**, W. Grundy, J. Hanley, G.E. Lindberg

PHYS 530. Studying CO_2 solvent properties by microwave spectroscopic investigation of vinyl fluoride...CO_2...CO_2 trimers. **D.B. Kannangara**, R.A. Peebles, S.A. Peebles, B.H. Pate

PHYS 531. Quantum mechanical studies of singlet and triplet chlorine-, bromine-, and iodine-containing fluorocarbenes. **T.J. Arledge**, J.M. Standard

PHYS 532. Implementation of GPU-accelerated molecular dynamics simulations of monoproline chiral interfaces. **C. Si**, N.M. Cann

PHYS 533. Spectroscopic and computational characterization of a new series of organoboron derivatives for use in Suzuki-Miyaura coupling reactions. **A. Dorris**, T. Vaughan, D.L. Mattern, N. Hammer

PHYS 534. Single molecule spectroscopic studies of squaraine-based donor–acceptor–donor (D-A-D) dyes. **L.A. Hunt**, J.N. Gayton, T. Rill, A. Huckaba, **L.E. McNamara**, J.H. Delcamp, N. Hammer

PHYS 535. Synthesis and photophysical characterization of bipyridyl hybrid oligomers: Examining mixed Furan-thiophene systems using spectroscopy and DFT methods. **A.E. Steen**, S. Nguyen, T.L. Ellington, G.S. Tschumper, D.L. Watkins, N. Hammer

PHYS 536. Can a photoexcited quinoline induce structural changes in a molecular system? **J.R. Hunt**, I. Demianets, J. Dawlaty, T.J. Williams

PHYS 537. Using attenuated total reflectance infrared spectroscopy to monitor changes in substrate upon binding to allosterically activated human liver pyruvate kinase. **R. Brenner**, C.J. Wurrey, A. Fenton

PHYS 538. Ion transport and dynamics in polymerized ionic liquids. **S. Spittle**, M.F. Heres, M. Chen, T.E. Long, J. Sangoro

PHYS 539. Origin of vibrational frequency shifts in strongly bound water clusters. **E. Knodel**, J. Heindel, D.P. Schofield

PHYS 540. Characterization of the photophysical properties of CCC-N-heterocyclic carbene platinum pincer complexes at the single molecule level. **S. Autry**, M. Zhang, E.V. Dornshuld, V. Dixet, T.K. Hollis, C.E. Webster, N. Hammer

PHYS 541. Chemistry in disks. **M. Ruaud**, U. Gorti

PHYS 542. Catalytic activity of platinum nanoparticles upon surface deposition. **M.C. Sherman**

PHYS 543. Plasmonic selective absorbers for all-metal optical power generation. **N. Hogan**, M.T. Sheldon

PHYS 544. Evaluation of enhanced sampling molecular dynamics methods for the creation of solid polymer electrolyte configurations. **L. Younger**, G.E. Lindberg

PHYS 545. Withdrawn

PHYS 546. Power conversion via unidirectional tunneling of plasmonic hot electrons. **S. Wu**, M. Sheldon

PHYS 547. Effect of conformational changes on triplet formation in a heavy heteroatom conjugated polymer: Single polymer molecules and molecular aggregates. **B. Datko**, Z. Fei, M.J. Heeney, J.K. Grey

PHYS 548. Manipulating ionic liquid self-assembly near solid surfaces. **R. Hayes**, K. House

PHYS 549. Real time study of molecular adsoprtion and transport at liposomes surfaces monitored by second harmonic generation. **P. Hamal**, H. Nguyen, R. Kumal, R.L. McCarley, L.H. Haber

PHYS 550. Unraveling the photo-dynamics of indigo. **R. Rodriguez**

PHYS 551. Preparation of nanofibers of cellulose from Tara Gum wastes production to the remotion of paracetamol as a emerging pollutant (EPs) in water. **S. Ponce**, A. Gutarra, M.S. Peresin, M. Chavarria

PHYS 552. Thermal and thermodynamic behavior of ionic liquids and molten salts with high thermal stability. **B. Siu**, C. Cassity, M. Soltani, M. Vo, J.H. Davis, K.N. West

PHYS 553. Withdrawn

PHYS 554. Preparation and characterization of microcapsulated red phosphorus and its thermal analysis based on non-isothermal kinetic approach. **L. Jie**

PHYS 555. Investigation of oxidation reaction products of 2-phenylethanol using synchrotron photoionization. **A. Otten**, M.L. Wooten, A. Medrano, G. Meloni

PHYS 556. Computational study of single-site catalysts: MgO-supported iridium complexes. **S. Zhang**, D.A. Dixon, B.C. Gates

PHYS 557. Graphene functionalization dynamics in the gas-phase and in solution. **R.M. Brinn**, K.Z. Rinaldi, N. Patel, A. Crowther

PHYS 558. Withdrawn

PHYS 559. Characterization of high-performance fuel injectors for pulsed gas expansions. **A.M. Prophet**, J. Winner, S.W. North, R. Sanchez-Gonzalez

PHYS 560. Tensor network wavefunction methods. **Y. Zhao**

PHYS 561. Mechanism of the loss of C_2H_4 and H_2O in protonated methionine. **J. Le**, J. Johnston, P.B. Armentrout

PHYS 562. Investigating the size-dependent vibrational properties of atomically precise nanostructures. **R. Dziatko**, A.N. Beecher, M. Greenberg, M.L. Steigerwald, J.S. Owen, A. Crowther

PHYS 563. Predicting phase diagrams via free energy based genetical algorithms. **T. Loeffler**, H. Chan, B. Narayanan, S. Sankaranarayanan

PHYS 564. Raman spectroscopic investigations of DNA-gold hybrid nanoclusters. **G.A. Halingten-Verville**, L. Sumner, K. Laughter, S. Chakraborty, N. Hammer

PHYS 565. Thermo-sensitive chromic materials using thermosensitive polymer and ionic liquids. **S. Gupta**, N. Matsumi

PHYS 566. Solution structure of FXI:FXI dimer and activation mechanism by thrombin: A molecular docking and MD refinement study. **D. Venkateswarlu**

PHYS 567. Investigating the interaction of aryl tetrazolones with anions. **E. Nord**, H. Zhou, S. Rayat

‡*Cooperative Cosponsorship*

PHYS 568. Elucidating the flexibility effects on the hydrodynamic volume of hetero-FRET probes using fluorescence correlation spectroscopy and time-resolved fluorescence anisotropy. **N. Anye**, H. Leopold, H. Lee, J. Schwarz, E.D. Sheets, A.A. Heikal

PHYS 569. Hypergeometic resummation of the Møller-Plesset perturbation series for strongly correlated systems. **A. Patel**, N. Abbas, C.E. Gonzalez, P. Ayers

PHYS 570. Motion of the calmodulin/ryanodine receptor complex determined using NMR residual dipolar coupling experiments and molecular dynamics simulations. L. Cooper, P. Grewe, S. Roman, **M.C. Zwier**

PHYS 571. New organic crystals for THz generation. **G.A. Valdivia-Berroeta**, D. Michaelis, J. Johnson

PHYS 572. Mechanism of loss of carbon monoxide and water from protonated methionine. **L. Miller**, B. Bruggeman, J. Johnston, P.B. Armentrout

PHYS 573. Synthesis of thermally stable, reversibly thermochromic ionic liquids. J.H. Davis, **M. Soltani**

PHYS 574. Investigating the thermal stability of halogen containing perarylphosphonium-based ionic liquids. J.H. Davis, **J. McCants**

PHYS 575. Local dynamics of polyisobutylene in solution: An all-atom molecular dynamics study. **H. Ponce**, M.M. Fuson

PHYS 576. Linear infrared and NMR spectroscopies for the determination of short peptide phi and psi angles. **M.A. Kubasik**, C. Foster-Spence, M.C. Rotondaro, J. Dickovick

PHYS 577. Ionic modification of carbon nanomaterials for altering their capacity for interactions with ionic liquids. J.H. Davis, **M. Vo**, M. Soltani

PHYS 578. Post-Marcus electronic transition dynamics via the generalized quantum master equation: A new approach. **E. Mulvihill**, A. Schubert, X. Sun, Y. Lai, E. Geva

PHYS 579. Which functional is best? Small molecule electron donors, electron paramagnetic resonance spectroscopy, and density functional theory. **C. Mallares**, K. Mardis

PHYS 580. Photochromic switching in the plasmonic field of gold nanoparticles. **W. Harmon**, C.J. Otolski, C.G. Elles

PHYS 581. Cationic porphyrin basicity and possible implications in photodynamic therapy. **M. Ballester**, K. Chamarti, L. Sanz

PHYS 582. Real-time electronic dynamics using time-dependent configuration interaction singles/doubles. **T.S. Nguyen**, J. Parkhill

PHYS 583. Porphyrin tautomerization of the 5, 15 dibromo 10, 20 diphenyl porphine and 5 bromo 10, 15, 20 triphenyl porphine using VT HNMR. **M. Ballester**, A. Sangermano, M. Mccloskey

PHYS 584. Investigating planarity of electron donor oligomer by comparison of EPR parameters obtained computationally and experimentally. **K. Wallace**, K.L. Mardis

PHYS 585. Withdrawn

PHYS 586. Detailed study of the formation of sugar derivatives produced from the UV irradiation of astrophysical ice analogs. **M. Nuevo**, G. Cooper, J.M. Saunders, C.E. Buffo, C.K. Materese, S.A. Sandford

PHYS 587. Quantum mechanical calculations on metal-bearing dicarbides and experimental spectroscopic verification. **D.T. Halfen**, M. Burton, N.J. Deyonker, D.J. Clouthier, L.M. Ziurys

PHYS 588. Chemical modeling studies of interstellar cyanomethanimine isomers. **D. Quan**, X. Zhang, E. Herbst, M.T. Webb

PHYS 589. Preparation, characterization and storage of water vapours highly enriched in its ortho-H_2O nuclear spin isomer. **P. Ayotte**, P. Turgeon, J. Vermette, I. Brault, X. Michaut, L. Philippe, M. Bertin, T. Putaud, J. Fillion, G. Alexandrowicz

PHYS 590. Basis set dependence of carbon dioxide polarizability and hyperpolarizability using ab initio methods. **R. Beil**, R.J. Hinde

PHYS 591. Direct vibrational energy transfer in monomeric water probed with ultrafast two dimensional IR spectroscopy. **H. Bian**

PHYS 592. Robust algorithm for reaction path finding and transition state optimization. **X.D. Yang**, P. Ayers

PHYS 593. Evaluation of the Ho + O β $HoO^+ + e^-$ chemi-ionization reaction enthalpy by guided ion beam tandem mass spectrometry and quantum chemistry theoretical methods. **C. Owen**, J. Kim, P.B. Armentrout

PHYS 594. Propargyl alcohol cyclization via synchrotron photoionization. **M. Farley**, G. Meloni

THURSDAY MORNING

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory
Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers, Presiding*

8:30 PHYS 595. Withdrawn

9:00 PHYS 596. Withdrawn

9:30 PHYS 597. Exact exchange-correlation potentials of two-electron systems and exact Fermi potentials. **V.N. Staroverov**, I.G. Ryabinkin, E. Ospadov

10:00 PHYS 598. Directly patching exchange-correlation energy in density functional theory. **C. Huang**

10:15 Intermission.

10:30 PHYS 599. Making high accuracy affordable through DFT. **G.A. Petersson**

10:45 PHYS 600. Unraveling the electronic structure of organic photovoltaic donors: Selecting density functionals through electron paramagnetic resonance parameter prediction. **K. Mardis**, J. Niklas, O. Poluektov, C. Mallares, K. Wallace

11:00 PHYS 601. Influence of intramolecular and intermolecular interactions on the sensitivity of energetic materials. **A.L. Shoaf**, C.A. Bayse

11:15 PHYS 602. Towards an Ab initio understanding of the hydrated electron: DFT-based molecular dynamics simulations of water anion clusters. C. Zho, **B.J. Schwartz**

11:30 PHYS 603. Modeling phase equilibria using CP2K software suite. **H. Goel**, N. Rai

11:45 PHYS 604. Utilizing advanced kinetic energy density based ingredients for novel local hybrid mixing functions. **J.W. Furness**, J. Sun

12:00 PHYS 605. Multireference density functional theory with generalized auxiliary systems for ground and excited states. **Z. Chen**, D. Zhang, Y. Jin, Y. Yang, N. Su, W. Yang

Section B
Ernest N. Morial Convention Center
Room 220

Chirality from Molecules to Materials

Electronic Dynamics

M. Caricato, P.H. Vaccaro, *Organizers*
J.R. Cheeseman, *Presiding*

8:30 PHYS 606. Electrons spin and chirality: From molecular spintronics to enantio-recognition. **R. Naaman**

9:10 PHYS 607. Withdrawn

9:50 PHYS 608. Electronic excitation spectra calculation of large systems with a tight-binding based simplified Tamm-Dancoff approximation (sTDA-xTB). **J. Seibert**, C. Bannwarth, S. Grimme
10:10 PHYS 609. FVNO++: Towards a reduced-scaling method for coupled cluster chiroptical properties. **A. Kumar**, T. Crawford

10:30 Intermission.

10:50 PHYS 610. Real-time time-dependent density functional theory for computing electronic circular dichroism band spectra. **X. Li**

11:30 PHYS 611. What can be learnt on gas phase chiral systems by using photoelectron circular dichroism? **L. Nahon**

12:10 Concluding Remarks.

Section C
Ernest N. Morial Convention Center
Room 221

Understanding the Complexity of the Nano/Bio Interface with Experiments & Computations

Nanoparticle-Surface Structure & Dynamics

F. Geiger, C.F. Landes, *Organizers*
P. Jungwirth, *Presiding*

8:30 PHYS 612. Computational analysis of the nano/bio interface. **Q. Cui**

9:00 PHYS 613. Investigating nanoparticle self-assembly at the nano-membrane interface. **Z. Cournia**

9:20 PHYS 614. Lipid corona formation from nanoparticle interactions with bilayers and membrane: Specific biological outcomes. **F. Geiger**

9:40 Intermission.

9:55 PHYS 615. Deciphering the interplay between ligand-receptor interactions and nanoparticle-cell interactions in lipid-mediated cell binding and uptake. **B.M. Reinhard**, F. Xu, B. Eshaghi, S. Gummuluru

10:25 PHYS 616. Nanoparticle-induced oxidation of the protein corona initiates an oxidative stress response in cells. **C.K. Payne**

10:55 PHYS 617. Nanotopographic control of cytoskeletal dynamics. **J.T. Fourkas**, W. Losert

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Interfaces & Ionic Liquid Nanoscience

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
K. Schroeder, *Presiding*

8:30 PHYS 618. Re-structuring of molten inorganic salts and ionic liquids around Nanoparticles: Stable colloidal solutions. **V. Kamysbayev**, V. Srivastava, D.V. Talapin

8:50 PHYS 619. Taking a close look at ionic liquid / support interfaces. **H. Steinruck**

9:25 PHYS 620. Ionic liquid structure in bulk and at interfaces. B. Wu, M. Zhao, M.S. Emerson, Y. Wang, **E. Castner**

9:45 PHYS 621. Structure and screening behaviour of ionic liquids under nanoconfinement. **C.S. Perez Martinez**, S. Perkin

10:05 Intermission.

10:20 PHYS 622. Probing the structure of an ionic liquid interface by reactive atom scattering. E.J. Smoll, S. Purcell, L. D'Andrea, J.M. Slattery, D.W. Bruce, M.L. Costen, K.G. McKendrick, **T.K. Minton**

10:40 PHYS 623. Following reactions in ionic liquids through the outer surface by X-ray photoelectron spectroscopy. **F. Maier**, H. Steinrueck

11:15 PHYS 624. Effect of the environmental humidity on the interfacial properties of Ionic liquids. **R.M. Espinosa-Marzal**

11:50 PHYS 625. Reversible, micron-scale ordering in ionic liquid films. **R.S. Anaredy**, R. Specht, S.K. Shaw

Section G
Ernest N. Morial Convention Center
Room 225

Quantum Chemistry, Dynamics &

‡*Cooperative Cosponsorship*

Reaction Modeling for Molecules & Materials in Astrophysical Environments

Modeling: ISM/Clouds & (Exo) Planetary Atmospheres

H. Cuppen, D.E. Woon, *Organizers, Presiding*

8:30 PHYS 626. Help is needed: Some current astrochemical problems. **E. Herbst**

9:05 PHYS 627. Astrochemical kinetic models of dark molecular clouds: Statistical methods and TMC-1. **D. Maffucci**, E. Herbst

9:25 PHYS 628. Deuterium fractionation from molecular clouds to protoplanetary disks: Modeling and observation. **L. Majumdar**

9:45 PHYS 629. The unusual dynamics and chemistry in planetary nebulae. **L.M. Ziurys**, D. Schmidt, L.N. Zack, N. Woolf

10:05 PHYS 630. Modeling the chemistry in the complex outflows of supergiant stars. **D. Schmidt**, G. Adande, L.M. Ziurys

10:25 Intermission.

10:45 PHYS 631. Atmospheric chemistry on Venus: An overview of unresolved issues. **F. Mills**, E. Marcq, Y. Yung, C. Parkinson, K. Jessup, A. Vandaele

11:20 PHYS 632. Modeling exoplanet atmospheric chemistry in the era of the James Webb Space Telescope. **S. Horst**

11:55 PHYS 633. From the rocky kernel to the exosphere: the journey of alkali in Europa. **Y. Ellinger**

Elucidation of Mechanisms & Kinetics on Surfaces
Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Unconventional Catalysis Targeting Stable Molecules
Sponsored by CATL, Cosponsored by ENFL, ENVR, INOR and PHYS

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

THURSDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Room 219

Adventures in Density Functional Theory
Cosponsored by COMP‡
P. Ayers, W. Yang, *Organizers*
J.L. Gazquez, *Presiding*

1:30 PHYS 634. Density based electron localization function. **A.E. Mattsson**

2:00 PHYS 635. From chemical information in semilocal functionals to correcting a functional. **J. Contreras-Garcia**

2:30 PHYS 636. Incorporating charge transfer directionality in a global and local charge transfer model. **A. Vela**, U. Orozco-Valencia, J.L. Gazquez

2:45 PHYS 637. The parabolic interpolation is justified by thermodynamics. **M. Franco-Pérez**, J.L. Gazquez, P. Ayers, A. Vela

3:00 PHYS 638. Conceptual DFT formulated general purpose reactivity indicator for predicting and classifying the reactivity of sites within a molecule. **J.S. Anderson**, P. Ayers

3:15 PHYS 639. Maximum hardness principle applied for solids: Systems, reactions, phenomena. **W. Grochala**

3:30 PHYS 640. Chemical transferability of functional groups follows from the nearsightedness of electronic matter. **S. Fias**, P.F. Geerlings, P. Ayers

3:45 Intermission.

4:00 PHYS 641. Variational information-theoretic atoms-in-molecules. **F. Heidar-Zadeh**, T. Verstraelen, E. Vohringer-Martinez, P. Bultinck, P. Ayers

4:30 PHYS 642. Theory and applications of density-base energy decomposition analysis (DEDA). **Q. Wu**

4:45 PHYS 643. Frustrated Lewis trios and long-range hole interactions. **J. Echeverria**

5:00 PHYS 644. Benchmarking density functional methods for calculation of state energies of first row spin-crossover molecules. **J. Cirera Fernandez**, E. Ruiz

5:15 PHYS 645. Systematic determination of Hubbard *U* for high-throughput DFT calculations. **J.W. Bennett**, S. Spurgeon, I. Metz, B. Hudson, S.E. Mason

5:30 PHYS 646. Simulating ionization-triggered attosecond charge migration with TDDFT. A. Bruner, A. Sissay, S. Hernandez, F. Mauger, P. Abanador, M. Gaarde, K. Schafer, **K. Lopata**

Section C
Ernest N. Morial Convention Center
Room 221

Understanding the Complexity of the Nano/Bio Interface with Experiments & Computations

Novel Methods

C.F. Landes, *Organizer*
F. Geiger, *Organizer, Presiding*

1:30 PHYS 647. Solving the needle in the haystack problem: Novel optical nanoprobes for characterizing the nano-bio interface. **R.J. Hamers**, M.E. Robinson, R.H. Goldsmith, E. Evans, O. Shenderova, J. Ng, K. Kim, J.A. Pedersen

2:00 PHYS 648. Probing interactions between synthetic nanoparticles and model systems of pulmonary surfactant by vibrational sum frequency generation spectroscopy. **Z. Lu**

2:20 PHYS 649. Second harmonic generation studies of nanoparticle-based drug-delivery systems. **L.H. Haber**, R. Kumal, R.A. Khoury, H. Nguyen, J.C. Ranasinghe, P. Hamal, A.S. Dikkumbura, H.T. Smith, R.L. McCarley

2:50 PHYS 650. Resolving interfacial protein dynamics by super temporal-resolved microscopy (STReM). **C.F. Landes**

3:10 Intermission.

3:25 PHYS 651. Visualizing catalytic enhancements at metal-metal interfaces and nano-gaps via correlated super-resolution and electron microscopy. **P. Chen**

3:55 PHYS 652. Cell penetration and membrane fusion: Two sides of the same coin. **P. Jungwirth**

4:15 PHYS 653. Characterizing the ligand structure and stoichiometry on quantum dots using NMR spectroscopy. C. Zhang, G. Palui, B. Zeng, **H.M. Mattoussi**

4:35 PHYS 654. Hydrogen bond populations and dynamics in sorbitan surfactant reverse micelles. **C.P. Baryiames**, E. Ma, C.R. Baiz

4:55 Concluding Remarks.

Section D
Ernest N. Morial Convention Center
Room 214

Physical Chemistry of Ionic Liquids

Ionic Liquid-Solute-Solvent Interactions

Cosponsored by COLL‡
Financially supported by U.S. Army Research Office
E. Castner, E. Maginn, C.J. Margulis, S.K. Shaw, J.F. Wishart, *Organizers*
F. Maier, *Presiding*

1:30 PHYS 655. First principles molecular dynamics study of a deep eutectic solvent: Choline chloride/urea and its mixture with water. E.O. Fetisov, D.B. Harwood, I.W. Kuo, S.E. Warrag, M.C. Kroon, C.J. Peters, **J.I. Siepmann**

1:50 PHYS 656. Ionic liquid nanostructure enables alcohol self assembly. **R. Atkin**, T. Murphy, R. Hayes, S. Imberti, G. Warr

2:25 PHYS 657. From cnidaria to mollusca: Bulk and surface structuration in ionic liquids. **J. Canongia Lopes**, K. Shimizu, A.A. Freitas

3:00 PHYS 658. Intermolecular interactions and vibrational perturbations in 1-ethyl-3-methylimidazolium thiocyanate/water mixtures. C.R. Hutchison, S.N. Johnson, C. Williams, N. Hammer, C.L. Hussey, **G.S. Tschumper**

3:20 Intermission.

3:35 PHYS 659. Surface-active ionic liquids in water: Targeted nanoreactors for synthesis, catalysis and materials preparation. **K. Schroeder**, A. Cognigni, M. Hejazifar, R. Zirbs, C. Schröder

4:10 PHYS 660. Structural organization in protic ionic liquid/molecular liquid mixtures. **A. Triolo**, O. Russina

4:30 PHYS 661. Impact of alcohol size and identity on the dynamics of an imidazolium-based ionic liquid. **T. Miller**, S. Corcelli

4:50 PHYS 662. Effect of gas impurities on the CO_2 uptake in superbase ionic liquids. **R. Taylor**, H. Daly, A. Greer, J. Jacquemin, C. Hardacre

5:10 Concluding Remarks.

Elucidation of Mechanisms & Kinetics on Surfaces
Sponsored by CATL, Cosponsored by COLL, ENVR and PHYS

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

POLY

Division of Polymer Chemistry

T. Epps, C. Lipscomb and B. Helms, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

How to Foster Diversity in the Chemical Sciences (see *CMA*, Mon)

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis (see *PMSE*, Tue, Wed)

Polymers with Complex Architecture: From Synthesis to Self-Assembly (see *PMSE*, Sun, Mon, Tue, Wed)

New Horizons in Sustainable Materials (see *CELL*, Sun)

Recent Advances in Particulate & Colloid Materials for Biomedical Applications (see *COLL*, Tue, Wed)

SUNDAY MORNING

Section A
New Orleans Marriott Canal Street
Studio 6

International Symposium on Biorelated Polymers: Tutorial
Cosponsored by PMSE
C. Scholz, *Organizer*
F. Wurm, *Organizer, Presiding*
M. Barz, *Presiding*

7:55 Introductory Remarks.

8:00 POLY 1. Designing polymers for controlled release applications. **K.E. Uhrich**

8:45 POLY 2. Targeting cancer using stimuli-sensitive polymeric micelle.. **S. Quader**, **K. Kataoka**

9:30 POLY 3. Modification of hydrophilic polyesters with fatty acids for drug release systems. **J. Kressler**, K. Maeder

10:00 Intermission.

10:30 POLY 4. Biomedical applications of nano-sized polymeric micelles and polyion complexes. **A.V. Kabanov**

11:15 POLY 5. Design of antioxidative nanomedicines. **Y. Nagasaki**

Section B
New Orleans Marriott Canal Street
Studio 1

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
Cosponsored by PHYS and PMSE
A. Mariani, J.A. Pojman, A. Taylor, *Organizers*
K.F. Fazende, *Presiding*

8:05 Introductory Remarks.

8:15 POLY 6. Nonlinear dynamics and

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polymer systems: An overview. I.R. Epstein, **J.A. Pojman**, A. Taylor

9:00 POLY 7. Withdrawn

9:30 POLY 8. Coupling nonlinear optical dynamics to polymer systems for light-directed evolution of morphology. S. Biria, **I.D. Hosein**

10:00 Intermission.

10:30 POLY 9. Autonomous non-linear chemical control of functional polymer vesicle self-assembly from a 'homogeneous mixture'. **B. Bastakoti**, J. Perez-Mercader

11:00 POLY 10. Out-of-equilibrium self-assemblies and autonomous material systems with programmable lifetimes. **A. Walther**

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

New Methods Development

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises

A.D. English, *Organizer*
H. Cheng, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 POLY 11. Development of polymeric MRI agents as theranostics. **K. Thurecht**, A. Fuchs, A. Bapat, Z. Houston

8:30 POLY 12. Characterization of hydrogels with NMR techniques. Y. Jia, C. Malveau, **J.X. Zhu**

8:55 POLY 13. Characterization of patchy nanoparticles by solid-state NMR. **L.G. Reven**, B. Guzman Juarez, K. Kim, A. Abdelaal, S. Allie, V. Toader

9:20 POLY 14. NMR, X-ray and electron crystallography for crystalline polymorphs and salt/cocrystal/continuum issues at natural abundance. **Y. Nishiyama**

9:45 Intermission.

10:00 POLY 15. Application of dipolar-filter based time domain NMR for probing molecular motions, polymer crystallization and polymerization kinetics. **E. Azevedo**

10:25 POLY 16. Integration of nuclear magnetic resonance spectroscopy with microfluidic devices: Materials and other challenges. **M. Utz**

10:50 POLY 17. Distribution of functional monomers in latex particles: PFGNMR study. **K. Beshah**

11:15 POLY 18. Quantitative analysis of polymers using sensitivity enhanced ^{13}C NMR spectroscopy. **J. Hou**, Y. He, S. Qiu, P. Sabatino

Section D
New Orleans Marriott Canal Street Studio 5

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
W.R. Gutekunst, C.K. Simocko, *Presiding*

8:00 POLY 19. High temperature metathesis polymerization: ADMET in the melt state of highly crystalline polymers. **M.H. Bell**, H. Hester, V. Gomez, A. Gallman, K.B. Wagener

8:20 POLY 20. Synthesis of AB and ABA type block copolymers by ring-opening metathesis polymerization of strained 1,9-paracyclophanedienes. **V. Komanduri**, D.R. Kumar, B. Lidster, M.L. Turner

8:40 POLY 21. Variable temperature ring-opening metathesis polymerization of cyclopentene and derivatives. **W.J. Neary**

9:00 POLY 22. Selective acyclic diene metathesis polymerization: New functional groups to create precise alternating and block polymers. **C.K. Simocko**, H. Rauf, H. Yahya, M. Horikawa, J. Chen

9:20 POLY 23. Ring-opening metathesis polymerization-induced self-assembly (ROMPISA) in both aqueous and organic media. **D. Wright**, M. Touve, L. Adamiak, N.C. Gianneschi

9:40 POLY 24. Triblock terpolymers by simultaneous tandem block polymerization. **K. Kluthe**, I. Freudensprung, **M. Klapper**

10:00 POLY 25. Modular functionalization of polymeric β-ketoesters *via* dynamic enamine chemistry. **M.B. Sims**, L. Bai, J.J. Lessard, B.S. Sumerlin

10:20 POLY 26. Clicking with living ROMP polymers. **W.R. Gutekunst**

10:40 POLY 27. Withdrawn

11:00 POLY 28. Multivariate study of the synthesis of sodium poly(styrene sulfonate) by aqueous atom transfer radical polymerization. **P. Balding**

11:20 POLY 29. Copolymerization of ethylene and polar olefins by heterobimetallic catalysts with phosphine-phosphonate ligands. **Z. Cai**, L. Do

11:40 POLY 30. Thio-bromo "click" approach for modifying materials prepared using ROMP. **C.E. Hobbs**

Section E
New Orleans Marriott Canal Street Studio 10

Polymer Applications & Characterization in Medical Device & Pharmaceutical Industries
Cosponsored by PMSE
Financially supported by Pfizer
J. Slager, *Organizer*
X.M. Liu, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 POLY 31. Ion exchange resins in pharmaceutical formulations and FloVitro™ biorelevant dissolution technology: A unique approach to studying biorelevant drug dissolution. **A. Gehris**

9:05 POLY 32. Drug delivery to the vessel wall with drug coated balloons. **J. Slager**

9:30 POLY 33. Use of high throughput methods in the discovery of novel excipient-solubilizers for drugs with low aqueous solubility. **T.H. Kalantar**, J. Zhao, M. Ladika, K. Harris, C.J. Tucker, M. Tulchinsky, S.J. Guillaudeu, T. Kuo, B. Bell, J. Kiefer, S. Chen, R.D. Krystosek

10:00 Intermission.

10:30 POLY 34. Enzyme responsive 5-flurouracil (5-FU) loaded hydrogels based on osalazine derivatives for colon-specific oral drug delivery. **M. Zhengang**, **M. Rui**, **Z. Sun***

11:00 POLY 35. Photograftable zwitterionic polymers resist cell and bacterial adhesion. **B. Leigh**, M. Hansen, A. Guymon

Section F
New Orleans Marriott Canal Street Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*
K.M. Miller, D.A. Savin, *Presiding*

8:00 POLY 36. Kinetic differences between primary, secondary, and tertiary alkyl thiols in thiol-ene reactions. **K. Long**, X. Zhang, S. Huang, J. Sinha, M. Podgorski, C. Bowman

8:20 POLY 37. Low energy fabrication of mixed matrix membranes through thiol-ene chemistry. **J.M. Schekman**, V. Vasagar, D. Bossier, S.I. Nazarenko

8:40 POLY 38. Withdrawn

9:00 POLY 39. Fabrication of luminescent quantum dot thiol-yne nanocomposites via UV photopolymerization. **D.A. Boyd**

9:30 POLY 40. Successful UV-Curing of epoxy composites. **S. Marco**, R. Liska, N. Klikovits

10:00 Intermission.

10:30 POLY 41. Substituent determined release from polymer microcapsules fabricated via thiol-ene photopolymerization. **D.V. Amato**, D. Amato, W. Martin, S. Swilley, M. Sandoz, D.L. Patton

10:50 POLY 42. Modified thiol-ene networks: Tuning the glass transition temperature and energy damping capabilities of photopolymerized networks. S. Godinez, O. McNair, K.C. Bentz, **D.A. Savin**

11:20 POLY 43. Development of vinyl sulfonate and vinyl sulfonamide: Its implementation in thiol-michael crosslinking polymerization. **J. Sinha**, M. Podgorski, C. Bowman

11:40 POLY 44. Thiol-ene 'click' poly(ionic liquid) networks: Correlating structure with conductive and gas separation properties. A.F. Bratton, S.P. Daymon, R.D. Johnson, H.B. Fannin, **K.M. Miller**

Section G
New Orleans Marriott Canal Street Beauregard

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
D.S. Germack, D.N. Haase, C. Lipscomb, J. Tsavalas, W. Wu, *Organizers*
J. Bohling, W. Gao, *Organizers, Presiding*

8:00 POLY 45. High biobased content latexes from plant oil-based vinyl monomers in miniemulsion. Z. Demchuk, K. Kingsley, I. Tarnavchyk, V. Kirianchuk, O. Shevchuk, A. Kohut, S. Voronov, **A.S. Voronov**

8:20 POLY 46. Microemulsion preparation of hollow silicone nanoparticles for incorporation in silicone hydrogels. **S.E. Morgan**, Q. Wu, A.L. Fogel

8:50 POLY 47. Improved latex stability made by a novel acrylic zwitterionic emulsion polymerization. **I. El-Hedok**, M. Ali, C. Lipscomb

9:20 POLY 48. Introduction to emulsion polymerization technology: Tutorial. **A.M. Maurice**

10:00 Intermission.

10:30 POLY 49. New developments in latex technology for coatings applications. **M.S. Ahmed**, D. Mestach, A. Steiner, F. Lunzer

11:00 POLY 50. Redox enhanced properties for emulsion polymers. **M. O Shaughnessy**

11:30 POLY 51. From soft latex particles to hard films: Synthetic routes towards achieving contradictory properties. **N. Ballard**, J. Asua

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

ACS Award in Applied Polymer Science: Symposium in honor Paula T. Hammond

Sponsored by PMSE, Cosponsored by POLY and WCC

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY AFTERNOON

Section A
New Orleans Marriott Canal Street Studio 6

International Symposium on Biorelated Polymers: Tutorial
Cosponsored by PMSE
F. Wurm, *Organizer*
C. Scholz, *Organizer, Presiding*
Y. Nagasaki, *Presiding*

1:00 POLY 52. Bicontinuous amphiphilic polymer co-networks. **G.N. Tew**

1:45 POLY 53. POZ™ –Poly(2-oxazoline) the next generation of polymer therapeutics. **R. Moreadith**

2:30 POLY 54. Polymer surfaces and

‡*Cooperative Cosponsorship*

graphene oxide anti-microbials. **R.C. Advincula**

3:00 Intermission.

3:30 POLY 55. Polypept(o)ides: Tailoring polymer properties for diagnosis and therapy. **M. Barz**

4:15 POLY 56. Poly(phosphoester)s: History, syntheses, degradation, bio-and flame-retardant applications. **F. Wurm**

Section B
New Orleans Marriott Canal Street Studio 1

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
Cosponsored by PHYS and PMSE
A. Mariani, J.A. Pojman, A. Taylor, *Organizers*
B. Thompson, *Presiding*

1:00 POLY 57. Autocatalysis in depolymerisation: degradation on demand. **A. Taylor**

1:30 POLY 58. Self-organization in precipitation reactions far from the equilibrium. **O. Steinbock**

2:00 POLY 59. DNA strand-displacement buffers. **D. Scalise**, R. Schulman

2:30 POLY 60. Non-equilibrium steady states in supramolecular polymerization. A. Sorrenti, J. Leira-Iglesias, A. Sato, **T.M. Hermans**

3:00 Intermission.

3:30 POLY 61. Designing highly thermostable biocatalysts. C. Choudhury, S. Tu, N. Yadavalli, N. Borodinov, S. Minko, I.A. Luzinov, **O. Kuksenok**

4:00 POLY 62. Controlling the evolution of frontal photopolymerization waves for 3D polymeric patterning. **A. Vitale**, M.G. Hennessy, O.K. Matar, J.T. Cabral

4:30 POLY 63. Potential reactants toward the synthesis of precipitation tubes. **J.J. Pagano**, C.B. Roys, M.J. Rase

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Supramolecules & Membranes

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
K. Saalwaechter, *Presiding*

1:00 POLY 64. The role of chirality in supramolecular organization. **H.W. Spiess**

1:25 POLY 65. Improving precision and stability of self-assembling supra-molecular materials using side chains with chiral centers. **R. Graf**

1:50 POLY 66. Solid-state dynamics of dipolar molecular rotors incorporated in supramolecular tripodal-triptycene assembly. **K. Yazawa**, F. Ishiwari, T. Fukushima

2:15 POLY 67. Measuring multi-scale tortuosity in polymer membranes. **L.A. Madsen**, A. Korovich, L.M. Thieu, L. Zhu, K. Chang, G.M. Geise, M.A. Hickner

2:40 Intermission.

2:55 POLY 68. Probing the hydrophilic domain structure and water transport in SDAPP proton exchange membranes. **T.M. Alam**, E.G. Sorte, C.H. Fujimoto, A.L. Frischknecht

3:20 POLY 69. Influence of hydrophobicity on dynamics of water in nano-meter scale space of polymer electrolyte membranes. **O. Han**

3:45 POLY 70. Understanding transport in polymeric separations membranes by combining NMR diffusometry and molecular dynamics simulations. **R. Zhang**, D. Troya, L.A. Madsen

4:10 POLY 71. Investigating multi-scale transport in random copolymer membranes for use in molecular separations. **A. Korovich**, K. Chang, T. Xue, W.A. Morris, L.A. Madsen, G.M. Geise

4:35 Intermission.
4:40 Panel Discussion.

Section D
New Orleans Marriott Canal Street Studio 5

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
A.M. Alb, B.S. Lokitz, *Presiding*

1:00 POLY 72. Electrical conductivity/ resistivity for copolymers carbon composites at cryogenically low temperature. **A. Aldalbahi**

1:20 POLY 73. nano-FTIR: Near-field spectroscopy of polymers at sub200ms per spectrum speed and sub20nm spatial resolution. **P. Schäfer**, T. Gokus

1:40 POLY 74. Applying multi-detector GPC/SEC to complex characterization of drug delivery polymers. **M.R. Pothecary**, C. Schindler, G. Zhang, H. Shen

2:00 POLY 75. Overcoming challenges in high molecular weight (HMW) polymer characterization. **A.M. Alb**

2:20 POLY 76. Network disassembly spectrometry with a non-degradable tracer: counting primary and secondary loops in polymer networks. **J. Wang**, T. Lin, Y. Gu, R. Wang, B.D. Olsen, J.A. Johnson

2:40 POLY 77. Probing the electromechanical response of ionic block copolymers using neutron reflectometry. **B.S. Lokitz**, J. Dugger, R. Kumar, W. Li, M. Chen, T.E. Long, J. Browning

3:00 POLY 78. Characterization of polymer brush properties using silicon photonic microring resonators. **S. Wetzler**, R.C. Bailey

3:20 POLY 79. Spectroscopic investigations of PS-PVDF blends. **E. Ibrahim**, M. Villarreal, M. Monayao, B. Adriana, D. Chipara, K. Lozano, M. Alcoutlabi, J. Hinthorne, M. Chipara

3:40 POLY 80. Effective characterization of oligomers and polymers by electrospray ionization with high-resolution mass spectrometry: New tool for lignomics. **A. Andrianova**, T. DiProspero, C. Geib, S. Reagen, I.P. Smoliakova, E. Kozliak, A. Kubatova

4:00 POLY 81. Temperature and solvent vapor switching properties of branched carbodiimde polymers. **E.H. De Silva**, C.U. Jayarathna, B.M. Novak

4:20 POLY 82. Route to low odor waterborne architectural coatings. **J. Bohling**, D. Lin, J. Xu, J. Zou, M. Gallagher, P. Doll

4:40 POLY 83. Withdrawn

Section E

New Orleans Marriott Canal Street Studio 10

Polymer Applications & Characterization in Medical Device & Pharmaceutical Industries
Cosponsored by PMSE
Financially supported by Pfizer
X.M. Liu, *Organizer*
J. Slager, *Organizer, Presiding*

1:00 POLY 84. Genomic DNA functionalized 3D printed materials for drug capture. **D. Yee**, M.D. Schulz, C. Blumenfeld, R.H. Grubbs, J.R. Greer

1:30 POLY 85. Pendent HDAC inhibitor SAHA derivatized polymer as a novel prodrug micellar carrier for anticancer drugs. **J. Xu**, J. Sun, S. Li

2:00 POLY 86. Conducting polymers as materials for wearable electronics and its application as biopotential electrodes. **S. Sinha**, Y. Noh, N. Reljin, Y. Guo, G. Treich, K. Chon, G. Sotzing

2:30 POLY 87. Surface modification of silicone catheters to combat device-associated complications. **K. Neoh**, M. Li, J. Bte Rahmat, M.K. Diwakar, E. Kang, E. Chiong, R. Wang

3:00 Intermission.

3:30 POLY 88. Design, synthesis and characterization of HPMA copolymer-niclosamide conjugates and its anticancer effect. **M. Rui**, **M. Zhengang**, **Z. Sun***

4:00 POLY 89. Small angle neutron scattering studies of gelatin as applied to liquid filled gelatin capsules. **J. Bachert**, **E. Chan**, B. Frieberg, R.L. Jones, B. Crawshaw, E. Maziarz, X.M. Liu

Section F
New Orleans Marriott Canal Street Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*
D.V. Amato, C. Ellison, *Presiding*

1:00 POLY 90. Photoinitiated copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) reaction for conductive network synthesis. **B. El-Zaatari**, A. Tibbits, C.J. Kloxin

1:20 POLY 91. Photopolymerizable and durable bio-based isosorbide resins for additive manufacturing. **D.N. Lastovickova**

1:40 POLY 92. Photoenforced surface segregation for the synthesis of gradient copolymers. **A. Vitale**, R.M. Bongiovanni

2:00 POLY 93. Living additive manufacturing with trithiocarbonate functionalized polymer networks. J. Lamb, Y. Gu, K. Qin, **J.A. Johnson**

2:30 POLY 94. High performance fibers via simultaneous spinning and photopolymerization. **C.J. Ellison**

3:00 Intermission.

3:30 POLY 95. Photoinitiated CuAAC–methacrylate-based interpenetrating polymer networks. **C.J. Kloxin**

4:00 POLY 96. Light-curable energetic binder synthesis and optimization DOE. **E. Cooke**, E.R. Beckel, A.J. Paraskos, M.N. Jablonski

4:20 POLY 97. UV curing technology – benefits, chemistries and trends. **A. Moeck**

4:40 POLY 98. Effect of molecular weight and degree of functionality on degradation, biocompatibility and 3-D printing of acrylated poly(caprolactone). **B. Green**, J. Thompson, K. Worthington, B. Tucker, A. Guymon

Section G
New Orleans Marriott Canal Street Beauregard

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
J. Bohling, W. Gao, D.S. Germack, C. Lipscomb, W. Wu, *Organizers*
D.N. Haase, J. Tsavalas, *Organizers, Presiding*

1:00 POLY 99. Nanocomposite microgels formed by seeded emulsion polymerization in the presence of radially structured polyelectrolyte microgels. **T. Watanabe**, S. Chihong, K. Murata, T. Kureha, D. Suzuki

1:20 POLY 100. Step-growth dispersion polymerization yielding monodisperse conjugated polymer particles for self-assembled organic lasers. **A.J. Kuehne**

1:40 POLY 101. Radical-mediated thiol-ene emulsion polymerizations. M.N. Arguien, K.J. Cassidy, D.V. Chapman, O.Z. Durham, **D.A. Shipp**

2:00 POLY 102. Polymer nanoparticles for drug delivery by PISA RAFT polymerization. **S. Perrier**

2:20 POLY 103. Polymerization-induced self-assembly in aqueous media: Tutorial. **S.P. Armes**

3:00 Intermission.

3:30 POLY 104. Layer-by-layer self-assembly of polyelectrolytic block copolymer worms on a planar substrate. **N.J. Penfold**, A. Parnell, M. Molina, P. Verstraete, J. Smets, S.P. Armes

3:50 POLY 105. One-pot synthesis of epoxy-functional amphiphilic diblock copolymer nano-objects from a single monomer via polymerisation-induced self-assembly. **F. Hatton**, S.P. Armes

4:10 POLY 106. Tuning the properties of worm gels prepared by RAFT dispersion polymerization in non-polar media. **M.J. Derry**, E. Raphael, S.P. Armes

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4:30 POLY 107. Exploring the formation and stability of Pickering emulsions stabilised by cross-linked diblock copolymer nanoparticles. **S.J. Hunter**, K. Thompson, J. Lovett, F. Hatton, C. Lindsay, S.P. Armes

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

ACS Award in Applied Polymer Science: Symposium in honor Paula T. Hammond

Sponsored by PMSE, Cosponsored by POLY and WCC

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

MONDAY MORNING

Section A
New Orleans Marriott Canal Street Studio 6

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Cosponsored by BIOT, MEDI and PMSE
M.B. Baker, R. Kieltyka, F.A. Leibfarth, *Organizers*
J.B. Matson, *Organizer, Presiding*
J. Barnes, *Presiding*

8:00 POLY 108. Supramolecular biomaterials enabling innovations in drug formulation and delivery. **E.A. Appel**

8:25 POLY 109. Nanofiber wound-dressings for treatment of multidrug-resistant infections. **C.L. McGann**, J. Lundin, L.A. Estrella, J.H. Wynne

8:45 POLY 110. Engineering intelligent hydrogel nanoparticles with tunable release properties. **A.M. Wagner**, N. Al-Sayyad, A.B. Shearer, N. Peppas

9:00 POLY 111. Tunable amino acid based biodegradable polyesteramides for drug delivery. **A.A. Dias**, J. Thies, G. Mihov

9:25 POLY 112. Brush-architectured poly(ethylene glycol) for oligonucleotide delivery. **K. Zhang**

9:45 POLY 113. Scalable ROMP polymers with drug delivery applications. **M. Golder**, J.A. Johnson

10:00 Intermission.

10:30 POLY 114. Glycopolymer probes to control immunity. **L.L. Kiessling**

10:55 POLY 115. Antifreeze-protein inspired polymers to enable (therapeutic) cell storage and distribution. C. Stubbs, B. Graham, T. Bailey, D. Fox, P. Scott, **M.I. Gibson**

11:15 POLY 116. Digital manufacturing for biomedical applications. **J. Poelma**, J. Rolland, E. Meyer

11:40 POLY 117. Polypept(o)ides: A novel class of biocompatible polymers based on endogenous amino acids. **M. Barz**

Section B
New Orleans Marriott Canal Street Studio 1

Integrating Polymer Science in the Curriculum
Cosponsored by CHED and PMSE
K.R. Carter, K.A. Cavicchi, S.E. Morgan, *Organizers*
K. Wingo, *Presiding*

8:00 POLY 118. Incorporating polymer science into the high school science classroom – NSF RET at the University of Southern Mississippi. **K. Wingo**, S.E. Morgan

8:15 POLY 119. Seeing the light in polymer science. **J. Sorrell**, B. Davis, Y.C. Simon

8:30 POLY 120. Incorporating polymer solar cell research in the high school classroom. **J. Brownlow**, M. Hall, V. Price-Walton, L. Moore, M. Woellner, S.E. Morgan

8:45 POLY 121. Polymers from potatoes: A Shark Tank challenge. **R.L. Lewis**, **R. Hooper**, V. Vasagar, R. Ramakrishnan, S.I. Nazarenko

9:00 POLY 122. Shape memory polymers in the classroom. **L. Ruttig**, K.A. Cavicchi

9:15 POLY 123. Classroom lesson on polymer molecular weight and dilute solution viscometry. **A. Cotugno**, N. Zacharia

9:30 POLY 124. Comparing and contrasting science and engineering through epoxy bridge building. **E. Schaub**, M.D. Soucek

9:45 POLY 125. Effect of the size and temperature of silver nanoparticles on their conductivity. **E. Polat**, A. Karim

10:00 Intermission.

10:30 POLY 126. Cross-linking the curriculum with polymer chemistry: A strategy to enhance polymer chemistry instruction in ACS-Certified Programs. **B.P. Quillian**, S.E. Gray, G. Guillet, C.W. Padgett, N. Shank, M. Weiland, S. Zingales

10:45 POLY 127. Preparing students for an industrial environment in a master's-level graduate internship program in polymer science. **D.R. Tyler**, S.E. York

11:00 POLY 128. INTERFACE: The National Science Foundation Graduate Research Traineeship Program at The University of Southern Mississippi. **D.L. Patton**, S.E. Morgan, K. Wingo

11:15 POLY 129. Expanding horizons: National Science Foundation NRT graduate student experiences at the University of Southern Mississippi. **A.L. Fogel**, A.N. Bristol, S.E. Morgan

11:30 POLY 130. Reflections and experiences of current and past NSF NRT Interface Trainees at the University of Southern Mississippi. **D. Amato**, **D.V. Amato**, **C.M. Reese**, **M. Vekasy**, D.L. Patton

11:45 POLY 131. Soft materials for life sciences: A National Science Foundation Graduate Traineeship Program. **K.R. Carter**

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Solid State Structure of Materials

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
J.L. White, *Presiding*

8:00 POLY 132. Solid-state NMR approaches to inorganic materials: From lead-halide perovskites to gallium phosphide. **L. Emsley**

8:25 POLY 133. Relations between amorphous and crystalline chain motions and the morphology of semicrystalline polymers. R. Kurz, M. Schaefer, A. Seidlitz, M. Schulz, T. Thurn-Albrecht, **K. Saalwaechter**

8:50 POLY 134. Chain tilt and crystallization of ethylene oxide oligomers with mid-chain defects. **D. Reichert**, Y. Golitsyn, M. Pulst, J. Kressler

9:15 POLY 135. Physical structures of semi-crystalline polymers in relation to their functional properties. **V.M. Litvinov**

9:40 POLY 136. Solid state dynamic nuclear polarization for materials study. **F. Aussenac**

10:05 Intermission.

10:20 POLY 137. Solid-state DNP NMR studies of crystalline polymer domains by co-polymerisation with radical monomers. H. Sardon, M.E. Verde, P. Ruiz, T. Huynh, D. Mecerreyes, M. Forsyth, **L. O'Dell**

10:45 POLY 138. Organic light-emitting diodes (OLEDs): Design-synthesis-fabrication, multiscale simulation, and DNP-NMR. **H. Kaji**

11:10 POLY 139. Structure determination of organic assemblies by magic angle spinning dynamic nuclear polarization. **G. De Paëpe**

Section D
New Orleans Marriott Canal Street Studio 5

Excellence in Graduate Polymer Research

Polymerization Techniques

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by POLY Industrial Advisory Board, Tosoh, and Wiley
C. Ellison, T.E. Long, *Organizers*
H. Cheng, C.J. Landry-Coltrain, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 POLY 140. Reversible control of polymer network topology using external light. **Y. Gu**, E. Alt, X. Li, A. Willard, J.A. Johnson

8:30 POLY 141. Utilizing polyaldehydes in designing optically degradable systems for transient technology. **A. Engler**, O. Phillips, J. Schwartz, G. Gourdin, P. Kohl

8:55 POLY 142. Photochemical regulation of redox-active catalysts: Controlling polyethylene microstructure with visible light. **J. Kaiser**, W. Anderson, B.K. Long

9:20 POLY 143. Material property evolution and mechanics during photopolymerization. **J. Wu**, Z. Zhao, C.M. Hamel, H. Qi

9:45 POLY 144. Mechanism-driven catalyst design for organocatalyzed atom transfer radical polymerization. **M.D. Ryan**, G. Miyake

10:10 Intermission.

10:25 POLY 145. Visible and NIR light photoinduced metal-free atom transfer radical polymerization. **C. Kütahya**, Y. Yagci, J. Gutmann, B. Strehmel

10:50 POLY 146. Neodymium-based catalysts $NdCl_3$-3L (L = triethyl phosphate (TEP) or tris(2-ethylhexyl) phosphate (TEHP) for ring opening polymerization of β-caprolactone. **Y. Ren**, R. Kularatne, K.E. Washington, M.C. Biewer, M.C. Stefan

11:15 Remarks by ACS President Peter K. Dorhout.

Section E
New Orleans Marriott Canal Street Studio 10

Industrial Innovations in Polymer Science
Cosponsored by I&EC
H.A. Brown, E.B. Murphy, *Organizers, Presiding*
M.B. Abrams, *Presiding*

8:10 Introductory Remarks.

8:20 POLY 147. Molecular design of olefin block copolymers and the impact on elastic performance in health and hygiene. **K. Anderson**, J. Lee, A. Stoiljkovic, J. Munro, L. Madenjian

8:40 POLY 148. Demands of the food industry for ever increasing material performance to meet the needs of today's consumers. **M.R. Watts**

9:00 POLY 149. Development of a fully automated small scale emulsion polymerization reactor. **R. Even**, G. Cardoen, L. Rhodes

9:20 POLY 150. Controlled aesthetics in thermoplastics: Modifying surface gloss of vinyl products. **K. Yocca**

9:40 POLY 151. A path to industry. **B. Zarin**

10:00 Intermission.

10:30 POLY 152. Extrusion replicated microcapillary film for managing condensation in food processing facilities. **K. Halverson**, S. Swanson, C. Nelson, D. Slama, J. Stratton, B. Martinez

10:50 POLY 153. Polyolefin contributions and new opportunities to meet societal and environmental needs. **P. Brant**

11:10 Concluding Remarks.

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Section F
New Orleans Marriott Canal Street Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*
A.J. Boydston, C. Boyer, *Presiding*

8:00 POLY 154. Visible-light driven RAFT polymerization accelerated by amines. **M. Allegrezza**, A. Kloster, Z. DeMartini, Z. Digby, D. Konkolewicz

8:20 POLY 155. Toward engineering macromolecular architectures of polymers through photoredox-mediated metal-free ring-opening metathesis polymerization. **P. Lu**, A.J. Boydston

8:40 POLY 156. Photoredox ring-opening polymerization of O-carboxyanhydrides to synthesize stereoblock polyesters. **R. Tong**

9:00 POLY 157. Photochemical control in ATRP. **K. Matyjaszewski**

9:30 POLY 158. Intramolecular charge transfer in organic photoredox catalysts for organocatalyzed atom transfer radical polymerization. **G. Miyake**

10:00 Intermission.

10:30 POLY 159. Mechanistic studies on photoredox-mediated metal-free ring-opening metathesis polymerization. **A.J. Boydston**

11:00 POLY 160. Using PET-RAFT for polymerization in low volume. **C. Boyer**

11:30 POLY 161. Rise and fall: Poly(phenyl vinyl ketone) photopolymerization and photodegradation under visible and UV radiation. **J.A. Reeves**, M. Allegrezza, D. Konkolewicz

Section G
New Orleans Marriott Canal Street Beauregard

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
J. Bohling, W. Gao, D.S. Germack, D.N. Haase, J. Tsavalas, *Organizers*
C. Lipscomb, W. Wu, *Organizers, Presiding*

8:00 POLY 162. RAFT emulsion polymerization: fundamentals and emerging materials. **Y. Luo**

8:30 POLY 163. Polymer-modified cellulose nanocrystals prepared by nitroxide-mediated polymerization and their use as CO_2-switchable Pickering emulsifiers. **J. Glasing**, J. Bouchard, P.G. Jessop, P. Champagne, M.F. Cunningham

8:50 POLY 164. Withdrawn

9:20 POLY 165. Stimuli-responsive nano-colloidals: Tutorial. **M.W. Urban**

10:00 Intermission.

10:30 POLY 166. Temperature and pH responsive colloidal diblock copolymer brushes prepared via SI-PIMP. L. Cao, K. Chen, **X. Guo**

10:50 POLY 167. Light-stimulated permanent shape reconfiguration in crosslinked polymer surfaces and microparticles. **L. Cox**, X. Sun, C. Wang, N. Sowan, J. Killgore, J. Xiao, R. Long, H. Wu, C. Bowman, **Y. Ding**

11:10 POLY 168. Control of particle shape and internal morphology: Polymer self-assembly and monomer feed based approaches. **P.B. Zetterlund**

11:40 POLY 169. *Ab-initio* emulsion ATRP by interfacial and ion-pair catalysis. **M. Fantin**, **K. Matyjaszewski**

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

ACS Award in Polymer Chemistry: Symposium in honor C. Grant Willson

Sponsored by PMSE, Cosponsored by POLY

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

MONDAY AFTERNOON

Section A
New Orleans Marriott Canal Street Studio 6

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Cosponsored by BIOT, MEDI and PMSE
M.B. Baker, R. Kieltyka, J.B. Matson, *Organizers*
F.A. Leibfarth, *Organizer, Presiding*
S. Radzinski, *Presiding*

1:00 POLY 170. Seek, destroy and heal: Enzyme-responsive nanoparticles as *In vivo* targeted delivery systems. **N.C. Gianneschi**

1:25 POLY 171. Thermoresponsive worms for expansion and release of human embryonic stem cells. **M. Monteiro**

1:45 POLY 172. Tuning release of signaling molecules by controlling mobility in a micelle core. **J.B. Matson**, J. Foster

2:10 POLY 173. Withdrawn

2:25 POLY 174. Nanostructural design, synthesis and characterization of antimicrobial and cytocompatible polymer surfaces. **K.J. Wynne**, C. Wang, O.Y. Zolotarskaya, X. Wen, D. Johnson

2:45 POLY 175. Bottlebrush nanoreactors for In situ synthesis. **J. Foster**, R.K. O'Reilly

3:00 Intermission.

3:30 POLY 176. Materials for drug capture: An approach to reducing the off-target toxicity of chemotherapy. **M.D. Schulz**, S. Oyola-Reynoso, S. Hetts

3:50 POLY 177. New polymer based approaches for biosensing and regenerative medicine. **M. Stevens**

4:15 POLY 178. Investigation of 1,2-oxazines: Dynamic covalent chemistry and structure-dependent thermal activation. **A.J. Boydston**, C. Lee, D. Church

4:40 POLY 179. Supramacromolecular strategy to combat multidrug-resistant bacteria. **J. Barnes**, X. Li, A. Delawder

Section B
New Orleans Marriott Canal Street Studio 1

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials

Frontal Polymerization

Cosponsored by PHYS and PMSE
A. Mariani, J.A. Pojman, A. Taylor, *Organizers*
D. McKenzie, *Presiding*

1:00 POLY 180. Frontal polymerization for art and rapid repairs. **J.A. Pojman**

1:25 POLY 181. Dual-cure initiating systems for photoinduced frontal cationic polymerization: application to carbon composite. **X. Allonas**, M. Lecompère, D. Maréchal, A. Criqui

1:50 POLY 182. Frontal polymerization of gels derived from dicyclopentadiene. **E.M. Lloyd**, L.M. Dean, E.B. Mejia, N.R. Sottos, J.S. Moore, S.R. White

2:15 POLY 183. Frontal ring-opening metathesis polymerization for rapid curing of fiber-reinforced composites. **L.M. Dean**, I. Robertson, M. Yourdkhani, P. Centellas, D. Ivanoff, J.S. Moore, S.R. White, N.R. Sottos

2:40 POLY 184. The effect of conductive material to modulate front velocities in self-propagating thermal frontal polymerization systems. J.A. Pojman, **C. Weber**

3:00 Intermission.

3:30 POLY 185. Frontal polymerization: A valuable method for obtaining functionally gradient materials. **G. Malucelli**, A. Mariani, D. Nuvoli, V. Alzari, J.A. Pojman

3:55 POLY 186. Behavior of acrylates forming deep-eutectic solvents in thermal frontal polymerizations by free radicals. **J.D. Mota-Morales**, K.F. Fazende, J.A. Pojman

4:20 POLY 187. Polymerization fronts in deep eutectic solvents. **I.A. Quintero**, J. Delgado

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Interfacial & Smart Systems

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises

H. Cheng, *Organizer*
A.D. English, *Organizer, Presiding*

1:00 POLY 188. Simple solids NMR experiments reveal routes to tailored interfaces in copolymers. **J.L. White**

1:25 POLY 189. New insights in bulk heterojunction interfacial structure from REDOR NMR. **R. Nieuwendaal**

1:50 POLY 190. Behavior of poly(styrene-co-methyl methacrylate-d_3) on silica. **F.D. Blum**, M. Maddumaarachchi, U.N. Arua

2:15 POLY 191. NMR assessment of structure and dynamics within metal organic frameworks. **J.A. Reimer**

2:40 Intermission.

2:55 POLY 192. Dynamical processes in self-healing hybrid polymer networks: A solid-state NMR study. **C. Lorthioir**, L. Rozes

3:20 POLY 193. Confined coil-to-globule transition of thermoresponsive polymers as revealed by solid-state NMR. F. Wang, **P. Sun**

3:45 POLY 194. Probe molecules for pulsed-field-gradient diffusion NMR experiments on micelles. **M.D. Lingwood**, B. Schepergerdes, M.S. Medrano, S.J. Bachofer

4:10 POLY 195. Compatibility evaluation of non-woven composite sheet based on silk fibroin and synthetic polymers for tissue engineered material. **Y. Nakazawa**, K. Numata, H. Tajiri, N. Hattori, D. Aytemiz, A. Asano, C.T. Nakazawa

Section D
New Orleans Marriott Canal Street Studio 5

Excellence in Graduate Polymer Research

Synthesis & New Materials

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by POLY Industrial Advisory Board, Tosoh, and Wiley
H. Cheng, T.E. Long, *Organizers*
C. Ellison, C.J. Landry-Coltrain, *Organizers, Presiding*

1:00 Recogntion of Poster Presenters.

1:15 POLY 196. Self-assembly of Pluronic triblock copolymers in a protic ionic liquid and polymerization to create wearable electronics. **R. Chen**, C. Lopez-Barron, N.J. Wagner

1:40 POLY 197. Biodegradable zwitterionic polylactide-based delivery systems for cancer treatment. **H. Sun**, Y. Wu, C. Cheng

2:05 POLY 198. Anionic ring-opening polymerization of azetidine. **L. Reisman**, E.A. Rowe, P. Rupar

2:30 POLY 199. High-spin ($S = 1$) conjugated copolymer with a paramagnetic ground-state. **A.E. London**, H. Chen, A. Sabuj, N. Rai, M.K. Bowman, J.D. Azoulay

2:55 Intermission.

3:10 POLY 200. Successive and chemoselective post-polymerization modification strategy. **T. Kubo**, C.A. Figg, J. Swartz, K.C. Bentz, K. Powell, M. Tansky, A. Chauhan, D.A. Savin, B.S. Sumerlin

3:35 POLY 201. Controlling the diffusion and solubility of water in epoxy/amine thermosetting polymers. **J. Vergara**, J.J. La Scala, C. Henry, J.M. Sadler, S.K.

‡*Cooperative Cosponsorship*

Yadav, G. Palmese

4:00 POLY 202. Structure-property relationships of novel (co)polyesters: From advanced packaging materials to the influence of regiochemistry on cyclics and properties. **R.J. Mondschein**, J.M. Dennis, H. Liu, R. Ramakrishnan, R.H. Colby, S.I. Nazarenko, S.R. Turner, T.E. Long

Section E
New Orleans Marriott Canal Street Studio 10

Industrial Innovations in Polymer Science
Cosponsored by I&EC
H.A. Brown, E.B. Murphy, *Organizers, Presiding*

1:00 Introductory Remarks.

1:10 POLY 203. Enzyme/polymer synergies: An innovative approach to sustainable detergents. **K.M. Knauer**, K.E. Gutowski, D. Hawker

1:30 POLY 204. Chronicling a sustainability journey in durable water repellent technology within the textile market segment. **G.O. Brown**, J.C. Sworen

1:50 Intermission.

2:00 POLY 205. Industrial R&D in functional polymer science: Cross-fertilization and food-water-energy nexus. A. Graillot, **C. Loubat**

2:20 POLY 206. Polymeric-based scale inhibitors for industrial water treatment applications. **K. Young**

2:40 POLY 207. Utilizing polymer chemistry to do more with less: Strategic approaches for more efficient oil well cementing. **M.G. Kellum**

3:00 Intermission.

3:30 POLY 208. Improving efficiency of making thermoset polymers: A new method for ambient cross-linking of polyethylene without heat, radiation, or moisture. **S. Sengupta**, J.M. Cogen, R. Mehta, M. Esseghir

3:50 POLY 209. Constitutionally dynamic polymers as oil well construction materials. **P. Boul**, D.K. Rasner, P.D. Jarowski, C.J. Thaemlitz

4:10 POLY 210. Development of chemistries to improve Guar Gum efficacy in hydraulic fracturing applications. **P. Abivin**, C.R. Hilliard, Y. Li, R. Prabhu, T. Kuo, C.W. Nelson, D. Khvostichenko, T. Austin, M. Rinken, S. Makarychev-Mikhailov

4:30 Concluding Remarks.

Section F
New Orleans Marriott Canal Street Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*
A. Anastasaki, J.J. Xu, *Presiding*

1:00 POLY 211. Photoinduced living polymerization for precision polymer synthesis. **J.J. Xu**

1:30 POLY 212. Exploiting light to push the limits of controlled radical polymerization. R.N. Carmean, C.A. Figg, G. Scheutz, T. Kubo, M.B. Sims, T. Becker, **B.S. Sumerlin**

2:00 POLY 213. Developments in aqueous copper(II) photoinduced polymerization of acrylates. **D.M. Haddleton**, G. Jones, R. Whitfield, A. Anastasaki

2:30 POLY 214. Shedding a light on state of the art photo-mediated controlled polymerizations. **A. Anastasaki**, N. Dolinski, I. Lee, C.J. Hawker

3:00 Intermission.

3:30 POLY 215. Photodisruptable layer-by-layer films. **S.W. Thomas**

4:00 POLY 216. Controlling macromolecular synthesis with different colors of light. **C. Barner-Kowollik**

4:30 POLY 217. Wavelength selective photochemistry for simultaneous multi-material printing. **Z.A. Page**, N. Dolinski, B. Callaway, F. Eisenreich, R. Garcia, R. Chavez, D. Bothman, S. Hecht PhD, F. Zok, C.J. Hawker

Section G
New Orleans Marriott Canal Street Beauregard

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
W. Gao, D.N. Haase, C. Lipscomb, J. Tsavalas, W. Wu, *Organizers*
J. Bohling, D.S. Germack, *Organizers, Presiding*

1:00 POLY 218. Monitoring of emulsion polymerization with ACOMP and early results on control. A. Wu, R.D. Montgomery, M.F. Drenski, T. McAfee, **W.F. Reed**

1:30 POLY 219. Mechanism of skin layer formation during drying of latex films. **H. Huang**, D. Ou-Yang, W. Lau, M.S. El-Aasser

1:50 POLY 220. Determination of charge distribution by electrical field-flow fractionation combined with multi-angle light scattering. **A. Meyer**, C. Johann, S. Elsenberg

2:20 POLY 221. Analysis of polymer colloids: Tutorial. **W. Gao**

3:00 Intermission.

3:30 POLY 222. Detection and characterization of single polymeric nanoparticles with surface plasmon resonance imaging microscopy. **R.M. Corn**

4:00 POLY 223. Finding order in glasses: Structures and dynamics of glass-forming polymer colloidal liquids under confinement. B. Zhang, **X. Cheng**

4:30 POLY 224. Utilization of DSC for polymer colloid morphology analysis. **A.K. Tripathi**, J. Tsavalas

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

ACS Award in Polymer Chemistry: Symposium in honor C. Grant Willson

Sponsored by PMSE, Cosponsored by POLY

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Lignin: From Fundamentals to New Materials & Applications

Fundamental Understanding of Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center Halls D/E

Sci-Mix

T.H. Epps, B. Helms, C. Lipscomb, *Organizers*

8:00–10:00

126, 140-142, 144, 196, 199-202, 204-205. See previous listings.

239-240, 244-245, 255, 257-259, 261, 310-312, 314, 326-330, 368, 378, 387, 393-394, 396-398, 400, 402-403, 436, 507-509, 515-517, 525, 537-538, 542, 545, 547, 550-555, 557-563, 566-572, 574, 578-580, 582-583, 641, 809. See subsequent listings.

TUESDAY MORNING

Section A
New Orleans Marriott Canal Street Studio 6

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Cosponsored by BIOT, MEDI and PMSE
M.B. Baker, R. Kieltyka, F.A. Leibfarth, J.B. Matson, *Organizers*
J. Foster, M.D. Schulz, *Presiding*

8:00 POLY 225. Transformation of natural products into functional polymer systems, with guidance by biomedical application targets. **K.L. Wooley**

8:25 POLY 226. Block copolymers of polylactones and poly(propylene fumarate) for 3D printed biological scaffolds. **S.R. Petersen**, J. Wilson, M. Becker

8:40 POLY 227. Development of new polymers for biofabrication: Hydrogels for 3D printing and resins for DLP. **M.B. Baker**

9:05 POLY 228. Hydrolysis-driven controlled drug delivery and tunable adhesive properties via novel therapeutic methacrylic monomers. **Z. Wright**, S.A. Sydlik, B. Holt

9:20 POLY 229. Proteins and polymers: Synergies in bioconjugates and structures. **D. Konkolewicz**, R.C. Page, G. Lorigan, I. Sahu, K. Burridge, M. Lucius, T. Wright, E. Clark, A. Craig, J. Berberich, J. Stewart, H. Fischesser

9:45 POLY 230. Elastin-like peptide nanoparticles for drug delivery to the brain. **J. Pille**, L. van Oppen, S. van Lith, I. Vialshin, R. Raave, D. Gerrits, S. Heskamp, W. Leenders, O. Boermann, R. Brock, J. Smeitink, J. van Hest

10:00 Intermission.

10:30 POLY 231. Bioerodible poly(acetal)-based networks as controlled release matrices. **D.N. Amato**, D.V. Amato, W. Martin, S. Swilley, M. Sandoz, D.L. Patton

10:45 POLY 232. Surface modification of living cells with synthetic polymer nano- and microparticles. **H.A. Klok**

11:10 POLY 233. Charging up cellulose and curdlan: Expanding the potential of polysaccharide based polyelectrolytes for therapeutic delivery applications. **B.L. Nichols**, K.J. Edgar

11:25 POLY 234. Thermoresponsive copolymers for immunotherapy applications. **F. Vohidov**, J.A. Johnson

11:40 POLY 235. Surface-eroding polyanhydrides from thiol-ene polymerizations: A versatile synthetic material for bio-applications. K.R. Tillman, K.L. Poetz, A. Witkowski, R. Meacham, **D.A. Shipp**

Section B
New Orleans Marriott Canal Street Studio 1

Undergraduate Research in Polymer Science
Cosponsored by CHED and PMSE
S.E. Morgan, S.I. Nazarenko, *Organizers*
H. Broadhead, *Organizer, Presiding*

8:00 Introductory Remarks.

8:15 POLY 236. Nontoxic oligomeric flame retardants from the bioacid, itaconic acid. **V. Hill**, B.A. Howell, Y. Daniel

8:30 POLY 237. Flame retardant properties of phosphorous esters from biobased diphenolic acid. **H.A. Fulco**, B.A. Howell

8:45 POLY 238. Shape-memory and self-healing polyanhydrides. **A. Witkowski**, R. Meacham, K.R. Tillman, D.A. Shipp

9:00 POLY 239. Controlling polymer solubility with Diels-Alder chemistry and LCST. **E. Wilborn**, C.G. Gregory, P.J. Costanzo

9:15 POLY 240. Microstructural changes in polyolefin thermoplastic elastomers affect elastic recovery and energy dissipation. **L.A. Maynard**, B. DeButts, J.R. Barone

9:30 POLY 241. Manipulation of molecular topology and composition using Diels-Alder chemistry. **M.S. Meyersohn**, S. Gosting, T. Colt, R. Rhoads, K. Barcus,

‡*Cooperative Cosponsorship*

M. Markmann, P.J. Costanzo

9:45 POLY 242. A pro-antimicrobial network via degradable acetals (PANDA) prepared via thiol-ene photopolymerization. **W. Martin**, D. Amato, D.V. Amato, O. Mavrodi, S. Swilley, K. Parsons, D. Mavrodi, D.L. Patton

10:00 Intermission.

10:30 POLY 243. Bio-based pro-antimicrobial networks synthesized via thiol-ene photopolymerization. **S. Swilley**, D.V. Amato, D.N. Amato, L. Blancett, O. Mavrodi, W. Martin, M. Sandoz, G. Shearer, D. Mavrodi, D.L. Patton

10:45 POLY 244. Surface free energy characterization of biofilm resistant monomers. **V. Ghebranious**, J. Carlisle, S. Oskin, E.B. Henry, W. Wei, T.B. Cavitt

11:00 POLY 245. Surface free energy characterization of an adhesin protein. **S. Oskin**, J. Carlisle, V. Ghebranious, T.B. Cavitt

11:15 POLY 246. Controlling nanoscale organization of thiophene-based conductive polymers with self-assembling peptides. **E.I. James**, L. Jenkins, A. Murphy

11:30 Concluding Remarks.

Section C
New Orleans Marriott Canal Street
Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Rubbers & Conducting Polymers

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
S. Kawahara, *Presiding*

8:00 POLY 247. Poly(3-alkylthiophenes): Chain packing, side chain ordering, and phase composition from solid-state NMR. **M. Hansen**

8:25 POLY 248. Molecular-level order, disorder, and interactions in conjugated polymers and blends from solid-state NMR. **B. Chmelka**, M. Reddy, M. Idso, M. Junk, D. Andrienko, M. Hansen

8:50 POLY 249. Structure and dynamics of proton-conducting materials *via* solid-state NMR. Z.B. Yan, G. Foran, A.R. MacIntosh, A.P. Young, D.H. Brouwer, **G.R. Goward**

9:15 POLY 250. Elucidation of stabilization pathways of atactic-polyacrylonitrile by solid-state NMR spectroscopy. **T. Miyoshi**

9:40 Intermission.

9:55 POLY 251. Characterizing the structure and dynamics of the rubber and tackifier in pressure sensitive adhesives. **M. McCormick**, Y. Zhang

10:20 POLY 252. Characterization of network structural motifs in siloxane elastomers using magnetic resonance. **A.M. Sawvel**, S.C. Chinn, M. Gee, A. Maiti, H. Mason, R.S. Maxwell, J.P. Lewicki

10:45 POLY 253. Structure of crosslinking junctions of network polymers through rubber state NMR spectroscopy. **S. Kawahara**

11:10 POLY 254. Sulfur-33 NMR of organosulfur compounds and polymers. **K. Yamada**

Section D
New Orleans Marriott Canal Street
Studio 5

Excellence in Graduate Polymer Research

Bio-Related Polymers

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by POLY Industrial Advisory Board, Tosoh, and Wiley
C. Ellison, T.E. Long, *Organizers*
H. Cheng, C.J. Landry-Coltrain, *Organizers, Presiding*

8:00 POLY 255. Synthesis of high-density molecular DNA brushes by direct grafting-through polymerization of oligonucleotides. **X. Tan**, H. Lu, Y. Sun, X. Chen, D. Wang, K. Zhang

8:25 POLY 256. Synthetic, functional thymidine-derived polydeoxyribonucleotide analogues from a six-membered cyclic phosphoester. **Y.T. Tsao**, T.H. Smith, K.L. Wooley

8:50 POLY 257. Correlating animal source to physical and functional properties of gelatin methacrylamide hydrogels. **A.T. Young**, M.A. Daniele

9:15 POLY 258. Assembly of protein assembly at bionanocomposite interphases. **A.M. Grant**, V.V. Tsukruk

9:40 POLY 259. Synthesis of polysaccharide ABA triblock copolymers by one-pot cross-metathesis ring-opening metathesis polymerization. **K. Arrington**, J. Chen, R.J. Mondschein, T.E. Long, K.J. Edgar, J.B. Matson

10:05 Intermission.

10:20 POLY 260. Magnetic field remotely controlled highly-selective biocatalysis. **A. Zakharchenko**, N. Guz, A. Jardji, S. Minko, E. Katz

10:45 POLY 261. Biodegradable polyester elastomers from bio-based lactones. **G. De Hoe**, M. Zumstein, B.J. Tiegs, J. Brutman, K.P. McNeill, M. Sander, G.W. Coates, M.A. Hillmyer

Section E
New Orleans Marriott Canal Street
Studio 7

Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Aleksandr Zhukhovitskiy & Jeremiah A. Johnson

J.A. Johnson, A.V. Zhukhovitskiy, *Organizers*
E. Pentzer, *Presiding*

8:00 POLY 262. Shape persistent bicyclic [2.2.2] and [2.2.1] building blocks for porous materials. **T.M. Swager**

8:30 POLY 263. From single-site catalysts and supramolecular assemblies to porous organic polymer (POPs): Bridging homogeneous and heterogeneous catalysis. **S.T. Nguyen**

9:00 POLY 264. Organic reactions inspired by the organometallic chemistry of gold. **D. Toste**

9:30 POLY 265. N-heterocyclic carbenes as ligands for metal surfaces. **C.M. Crudden**

10:00 Intermission.

10:30 POLY 266. External control in ATRP. **K. Matyjaszewski**

11:00 POLY 267. Award Address (Nobel Laureate Signature Award for Graduate Education in Chemistry Sponsored by Avantor™ Performance Materials Inc.). Johnson group research in the post-Zhukhovitskiy era: Extremely stable NHC-functionalized gold nanorods and polyMOCs that switch between phantom and affine behavior. M. Macleod, Y. Gu, **J.A. Johnson**

11:30 POLY 268. Award Address (Nobel Laureate Signature Award for Graduate Education in Chemistry Sponsored by Avantor™ Performance Materials, Inc). New frontiers for carbenes and metal-organic cages in surface and polymer chemistry. **A.V. Zhukhovitskiy**, I.J. Kobylianskii, D. Toste, J.A. Johnson

Section F
New Orleans Marriott Canal Street
Studio 10

Polymer Networks: Soft Gels to Stiff Networks
Cosponsored by PHYS, PMSE and SOCED
E. Chan, R.B. Moore, *Organizers*
S. Kundu, *Organizer, Presiding*

8:00 POLY 269. Biomolecules for non-biological things: Materials construction through peptide design and solution assembly. **D.J. Pochan**

8:30 POLY 270. Bio-inspired glycopolymer hydrogels for biomedical applications. **S.E. Morgan**, A. Fogel, B.S. Upadhyay, K.A. Stockmal, P.K. Das

9:00 POLY 271. Molecularly imprinted super-aptamer hydrogels for RNA and DNA biosensors. **D. Spivak**, B. Hebert

9:20 POLY 272. β-Sheet nanocrystal-reinforced supramolecular elastomers. **L. Jia**

9:40 POLY 273. Redox-responsive artificial molecular muscles. **J. Barnes**, A.F. Greene, M. Danielson, K.P. Liles, A. Delawder

10:00 Intermission.

10:30 POLY 274. From cartilages to mussel glues: Extreme properties by network design. **X. Zhao**

11:00 POLY 275. Finding value of lignin through chemical and physical cross-linking for versatile applications. N.A. Nguyen, M. Cui, K. Meek, S.H. Barnes, C.C. Bowland, J.K. Keum, **A.K. Naskar**

11:30 POLY 276. Aqueous toughening in crosslinked marine animal proteins. **A.M. Grant**, M. Krecker, S. Tadepalli, M. Gupta, M. Crosby, P. Dennis, S. Singamaneni, R.R. Naik, V.V. Tsukruk

11:50 POLY 277. Structural evolution of thermoreversible triblock terpolypeptoid hydrogels undergo sol-gel transition. **N. Jiang**, G.L. Sternhagen, T. Yu, S. Xuan, Y. Zhang, V.T. John, D. Zhang

Section G
New Orleans Marriott Canal Street
Beauregard

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
F. Horkay, M. Kovaliov, *Presiding*

8:00 POLY 278. Brush-first ring-opening metathesis polymerization as a modular and scalable strategy for combination cancer therapy and molecular imaging. **H.V. Nguyen**, N. Gallagher, F. Vohidov, Y. Jiang, K. Kawamoto, H. Zhang, J.C. Barnes, A. Rajca, J.A. Johnson

8:20 POLY 279. "Polysoaps" via RAFT copolymerization forming well-defined, unimeric micelles for water remediation and targeted drug delivery: An old concept with contemporary relevance. **P.D. Pickett**, M.A. Dearborn, K. Stevens, C.L. McCormick

8:40 POLY 280. Synthesis,photophysical and biological studies on conjugated PPE type zwitterionic polymer. **Y. Yang**, K.S. Schanze

9:00 POLY 281. Swelling pressure and compressive behavior of cartilage polymers. **F. Horkay**, P.J. Basser

9:20 POLY 282. Synthesis of novel water soluble semiconducting polyrhodamine. **R.W. Wahalathantrige Don**, C. Scott

9:40 POLY 283. Directed reverse micelle self-assembly of branched amphiphiles: Effect of polymer architecture on aggregation behavior. **K. Kosakowska**, B. Myers, L.B. Lawson, J. Albert, S.M. Grayson

10:00 POLY 284. Polynitroxides to protect against bacterial biofilms. **N.R. Boase**, C. De La Fuente-Nunez, C. Lang, R.E. Hancock, K.E. Fairfull-Smith

10:20 POLY 285. Synthesis of lipase polymer hybrids via the grafting-from approach. **M. Kovaliov**, M. Allegrezza, D. Konkolewicz, S. Averick

10:40 POLY 286. Thermotropic one-handed spiralization of polyacetylenes based on main-chain conformation change from *Cis-transoid* to *Cis-Cisoid*. **L. Lijia**, Y. Wang

11:00 POLY 287. Loop control of gel mechanics. **Y. Gu**, K. Kawamoto, M. Zhong, M. Chen, L. Korley, M.J. Hore, J.A. Johnson

11:20 POLY 288. Unique aqueous self-assembly behavior of a new thermoresponsive diblock copolymer. **S. Byard**, M.J. Derry, M. Williams, R. Kontzedaki, A. Blanazs, S.P. Armes

11:40 POLY 289. Polybenzoxazine based on phenol and *m*-amino phenyl boronic acid. **H. Ipek**, J. Hacaloğlu

Section H
New Orleans Marriott Canal Street
Audubon

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
J. Bohling, D.S. Germack, C. Lipscomb, J.

‡*Cooperative Cosponsorship*

Tsavalas, W. Wu, *Organizers*
W. Gao, D.N. Haase, *Organizers, Presiding*

8:00 POLY 290. Determining the core, corona, and total size of CdSeS/ZnS quantum dots by SEC/QELS and TEM. **A.M. Striegel**, L. Pitkanen

8:30 POLY 291. Synthesis, characterization and some of applications of colloidal microgels from amino acids. **N. Sahiner**, S. Demirci

9:00 POLY 292. LC-MS studies of serum phase chemistry and interfacial behavior of aqueous oligomers during emulsion polymerization. **T. Zhang**, B. McCulloch, W. Gao, R. Even

9:30 POLY 293. Polypeptide composite particles. **P. Russo**, C. Rosu, A.M. Blake, S.S. Balamurugan

10:00 Intermission.

10:30 POLY 294. Investigating the effect of ionic group location in the self-assemblies of sequence-defined peptoid block copolymers. **G.L. Sternhagen**, S. Gupta, G. Schneider, Y. Zhang, V.T. John, D. Zhang

10:55 POLY 295. Withdrawn

11:15 POLY 296. Control of self-assembly of amphiphilic statistical copolymers by their composition. **T. NEal**, M.W. Murray, S.P. Armes, S. Spain, O. Mykhaylyk

11:40 POLY 297. Polymer, particle, vesicle? The new challenge for analytical separation technologies in polymer characterization. **R. Reed**, B. Sabagh, P. Clarke

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

Lignin: From Fundamentals to New Materials & Applications

Advances in Lignin Characterization

Sponsored by CELL, Cosponsored by ENVR and POLY

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

TUESDAY AFTERNOON

Section A
New Orleans Marriott Canal Street
Studio 6

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Cosponsored by BIOT, MEDI and PMSE
M.B. Baker, R. Kieltyka, F.A. Leibfarth, J.B. Matson, *Organizers*
M. Baker, M. Golder, *Presiding*

1:00 POLY 298. Shear-thinning and self-healing hydrogels for therapeutic delivery. **J.A. Burdick**

1:25 POLY 299. Glycosidase inhbition by "sweet" bottlebrush polymers. **E. Sletten**, R. Loka, H.M. Nguyen

1:40 POLY 300. Development of polymer theranostics to probe the behaviour of nanomaterials in biology. **K. Thurecht**, Y. Zhou, N. Fletcher, Z. Houston

2:05 POLY 301. Withdrawn

2:20 POLY 302. Phase-separating biopolymer conjugates to manipulate cell signaling and healing in cardiovascular tissues. **K.L. Kiick**

2:45 POLY 303. Catechol-functionalized bioinspired synthetic adhesives: Effect of comonomer on mechanical properties. **S. Radzinski**, M. Bartucci, D. Flanagan, J. Lenhart, J.A. Orlicki

3:00 Intermission.

3:30 POLY 304. Biodegradable blockcopolymers as drug carriers in cancer therapy. **M. Klapper**, F. Karagoez

3:50 POLY 305. Partially fluorinated polymers for spatiotemporal mapping of tissue oxygenation. **F.A. Leibfarth**

4:15 POLY 306. Elucidation of glycopolymer aggregation mechanism for determination of structure/binding interactions with amyloid β peptides. **A.N. Bristol**, P.K. Das, D.N. Dean, V. Rangachari, S.E. Morgan

4:30 POLY 307. Monodisperse fucosylated glycooligomers to investigate multivalent binding to LecB. **K. Buecher**, L. Hartmann

4:45 POLY 308. Bio-degradable conjugated polymer particles as biomedical imaging probes. **A.J. Kuehne**

Section B
New Orleans Marriott Canal Street
Studio 1

Undergraduate Research in Polymer Science
Cosponsored by CHED and PMSE
H. Broadhead, S.E. Morgan, *Organizers*
S.I. Nazarenko, *Organizer, Presiding*

1:00 POLY 309. Self-assembly of uniform nano pores for membrane transfer to silicon. **D.F. Ehlenberg**, X. Gu, D. Weller

1:15 POLY 310. Synthesis and structural investigation of customizable polyelectrolyte complexes. **A. Herzog-Arbeitman**, J.M. Ting, H. Wu, O. Werba, S. Srivastava, M.V. Tirrell

1:30 POLY 311. Self-healing polyelectrolyte/metal ion materials. **L. Mihlbachler**, H. Zhang, N. Zacharia

1:45 POLY 312. MoS_2 dispersed epoxy vitrimer composite: Role of solvent and surface chemistry of MoS2 on network formation, mechanics, and stimuli response. **I. Barrett**, J. Ryan, G. Kedziora, J. Moller, R. Berry, D. Nepal

2:00 POLY 313. Rational design of sensitive and selective conjugated polymer based fluorescent sensors for the detection of phosphate. **E. Crater**, A.K. Williams, J. Tropp, J.D. Azoulay

2:15 POLY 314. Novel binder development in binder jet additive manufacturing to improve green part strength. **D. Gilmer**, E. Hong, D. Siddel, A. Merriman, A. Kisliuk, S. Cheng, A. Elliott, **T. Saito**

2:30 POLY 315. Scavenging ruthenium in ring-opening metathesis polymerization-based branched polymers. M. Golder, H.V. Nguyen, **J. Grundler**, E. Park, J.A. Johnson

2:45 POLY 316. Synthesis of hyperbranched polymers with post-functionalization specificity. **H. Naguib**, X. Cao, H. Gao

3:00 Intermission.
4:10 Panel Discussion.

Section C
New Orleans Marriott Canal Street
Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Electrolytes & Polyelectrolytes

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
L.A. Madsen, *Presiding*

1:00 POLY 317. Liquid and solid state NMR investigations of low MW Polyether and non-polyether polymer electrolytes for supercapacitor and battery applications. **S. Greenbaum**, M. Gobet, J. Peng, S. Munoz, D. Morales, L. Carbone, J. Hassoun, R.E. Ruther, J. Nanda, M. Zimmerman, R. Leising

1:25 POLY 318. Solid-state NMR investigation of the solid electrolyte interphase on silicon electrodes for lithium ion batteries. **P. Magusin**

1:50 POLY 319. NMR studies of dynamical couplings in ionic liquids and polymer electrolytes. **M. Vogel**, M. Becher

2:15 POLY 320. Towards understanding the ionic conduction in solid state polymer electrolytes–a solid-state NMR study of PEO/Li^+ complex. **Y. Yao**

2:40 POLY 321. Studying ion transport in polymer electrolytes by NMR methods. **M. Schönhoff**

3:05 Intermission.

3:20 POLY 322. Understanding ion dynamics in conducting polyelectrolytes from angstroms to millimeters. **V. Witherspoon**, R. Nieuwendaal, J.L. Schaefer, C.M. Stafford, C. Soles

3:45 POLY 323. Ion dynamics in solid polymer blend electrolytes via inversion of the laplace transform. **L. Smith**, S. Granados Focil

4:10 POLY 324. Solid state ^{13}C NMR study of ethylene ionomers: Crystalline phase after heat treatment. **A. Asano**, T. Matsukawa, C.T. Nakazawa

Section D
New Orleans Marriott Canal Street
Studio 5

Excellence in Graduate Polymer Research

New Products & Characterization

Cosponsored by PRES, PROF, SOCED and YCC
Financially supported by POLY Industrial Advisory Board, Tosoh, and Wiley
C.J. Landry-Coltrain, T.E. Long, *Organizers*
H. Cheng, C. Ellison, *Organizers, Presiding*

1:00 POLY 325. Insights into the assembly of polyelectrolyte multilayers and complexes. **H.M. Fares**, J.B. Schlenoff

1:25 POLY 326. Thermal transitions in hydrated PDADMA–PSS complexes. **Y. Zhang**, P. Batys, M. Sammalkorpi, J.L. Lutkenhaus

1:50 POLY 327. Smart epoxy nanofiltration membranes for multicomponent separations. **C. Gilmer**, N.B. Bowden

2:15 POLY 328. Biomineralization-inspired mineral coating for nanofiber adsorbents development. **Y. Park**, E. Ford, T. Gardner

2:40 Intermission.

2:55 POLY 329. CNT 'trapping' via non-solvent induced phase separation. **H. Li**, M. Minus

3:20 POLY 330. Wetting transition on metamorphic superomniphobic surfaces. W. Wang, J. Salazar, **H. Vahabi**, A. Joshi-Imre, W. Voit, A. Kota

3:45 POLY 331. Understanding of polymer crystallization at the molecular scale: Topology, kinetics, and molecular weight effects. **S. Wang**, S. Yuan, T. Miyoshi

4:10 Career Panel.

Section E
New Orleans Marriott Canal Street
Studio 7

Adaptive Nanogels
Cosponsored by COLL
A. Fernandez-Nieves, L.A. Lyon, W. Richtering, D. Suzuki, *Organizers*
T. Hoare, *Organizer, Presiding*
A. Pich, *Presiding*

1:00 POLY 332. Adaptive nanogels as nanocapsule shells. **K. Landfester**

1:30 POLY 333. Withdrawn

2:00 POLY 334. Adaptable synthetic polymers as protein and peptide affinity ligands. An alternative to the lock and key paradigm. **K.J. Shea**

2:30 POLY 335. Aqueous microgels as reference beads for mass cytometry and supports for enzyme reactions at elevated temperatures. **M. Winnik**

3:00 Intermission.

3:30 POLY 336. Tuning pKa of Brønsted acids in temperature-responsive hydroel particles by proton- and ion-imprinting strategy. **Y. Hoshino**

4:00 POLY 337. Microgels as building blocks for tissue regenerative materials. **L. De Laporte**, L.P. Guerzoni, J.C. Rose, D. Gehlen

4:20 POLY 338. Electrochemically-active iron-containing microgels. **F. Plamper**, P. van Rijn, O. Mergel, S. Schneider

4:40 POLY 339. Polyelectrolyte and polyampholyte nanogels: Effect of electrostatics on internal structure, uptake and release of guest-molecules. A. Rudov,

‡*Cooperative Cosponsorship*

I. Portnov, A. Pich, W. Richtering, **I. Potemkin**

Section F
New Orleans Marriott Canal Street Studio 10

Polymer Networks: Soft Gels to Stiff Networks
Cosponsored by PHYS, PMSE and SOCED
E. Chan, S. Kundu, *Organizers*
R.B. Moore, *Organizer, Presiding*

1:00 POLY 340. Shear and cavitation rheology of polymer organogels. K.C. Bentz, N. Sultan, S. Walley, **D.A. Savin**

1:30 POLY 341. Rate dependent mechanics of crosslinked polymers. **J.L. Lenhart**, T. Long, D. Knorr, K. Masser, T.W. Sirk, R. Mrozek, J. Andzelm, E. Bain

2:00 POLY 342. Fracture of soft but solvent-free polymer networks. J. Sarapas, E. Rettner, K. Beers, **E. Chan**

2:20 POLY 343. Mechanical properties and failure behavior of alginate hydrogels. **S. Kundu**, S. Hashemnejad, R. Wijayapala, R. Badani Prado, S. Mishra

2:40 POLY 344. Hybrid particle-field approach for simulating inhomogeneous supramolecular polymer networks. **D. Meng**, J. Zong

3:00 Intermission.

3:30 POLY 345. Characterization of the transient networks formed by oligocarbonate-functionalized PEG block polymers. **V. Prabhu**

4:00 POLY 346. Molecular insights into early stage aggregation of molecular mass organic gelators. **N. Rai**, M. Huda

4:30 POLY 347. Can percolation theory account for the aqueous gelation behavior of diblock copolymer worms? **J. Lovett**, M.J. Derry, P. Yang, S.P. Armes

4:50 POLY 348. The role of chain extender in controlling the kinetics of morphology development of polyurethane elastomers. X. Tao, O. Wamuo, W. Zhao, **S.L. Hsu**

Section G
New Orleans Marriott Canal Street Beauregard

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
A. Karim, D. Siefker, *Presiding*

1:00 POLY 349. Soluble polymer-supported bidentate sulfur ligand for metal sequestering. **H. Bazzi**, D. Chouikhi, M. Al-Hashimi, D.E. Bergbreiter

1:20 POLY 350. Enhancing the selectivity of addition-type polynorbornenes for post-combustion carbon dioxide sequestration. **C. Maroon**, K.R. Gmernicki, N. Belov, Y.P. Yampolskii, S.M. Mahurin, T. Saito, **B.K. Long**

1:40 POLY 351. Accessing functional materials through organocatalyzed post-polymerization modification. **C.P. Easterling**, T. Kubo, Z.M. Orr, J.E. Sanchez, G.E. Fanucci, B.S. Sumerlin

2:00 POLY 352. Ionenes inspired by high-performane and ultra-high performance polymers. **K.E. O'Harra**, E.M. Devriese, D.M. Noll, G.P. Dennis, M.M. Durbin, E.M. Jackson, J.E. Bara

2:20 POLY 353. Reinforcement of industrial chloroprene rubber by polychloroprene grafted silica nanoparticles. **Z.M. Abbas**, M.M. Mohammadkhani, B.C. Benicewicz

2:40 POLY 354. Facile preparation of a free-standing hydrogen-bonded ladder polymer film. **T. Yuan**, X. Ji, M. Vazquez, L. Fang

3:00 POLY 355. Air-friendly synthesis of well-defined polypeptides by ring-opening polymerization of amino-acid derived N-thiocarboxyanhydrides. **D. Siefker**, J. Cao, D. Zhang

3:20 POLY 356. Impact of alkyne unsaturation on the flame retardant behavior of simple phosphorus diesters. **E. Ostrander**

3:40 POLY 357. Solvent-free formation of functional polymers by repurposing sulfur. C. Westerman, C. Perez, K. Kamp, **C. Jenkins**

4:00 POLY 358. 1-Dopyl-1,2-(4-hydroxyphenyl)ethene as a flame retardant curing agent for epoxy. **G.W. Lienhart**, B.A. Howell

4:20 POLY 359. Design and synthesis of highly stable triblock copolymers for anion exchange membrane fuel cells. **O. Ozcalik**, M.L. Anthamatten

4:40 POLY 360. Poly(vinylidene fluoride) based nanocomposites: Dielectric, piezoelectric, and pressure sensing characteristics. **M.K. Hassan**, A.A. Issa, A. Al-Saygh, D. Ponnamma, M.A. Al-Maadeed, A.S. Luyt

Section H
New Orleans Marriott Canal Street Audubon

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
J. Bohling, W. Gao, D.S. Germack, C. Lipscomb, J. Tsavalas, *Organizers*
D.N. Haase, W. Wu, *Organizers, Presiding*

1:00 POLY 361. Tutorial on modeling multi-phase polymer particle morphology development: Critical role of diffusion. **J. Tsavalas**, A.K. Tripathi, P. Zhang, R.H. Carrier, D.C. Sundberg

1:40 POLY 362. Calculation of oxygen-centered radical reaction rates in emulsion polymerization processes. J.M. Martinez, I. Konstantinov, **S.G. Arturo**, G. Dombrowski

2:00 POLY 363. Self-assembly dynamics and inner morphology of hydrophobically modified hyaluronic acid nanoparticles: Towards design of optimized drug nanocarriers. **D. Svechkarev**, A. Kyrychenko, W. Payne, A. Mohs

2:30 POLY 364. Real-time control and optimization: Demonstration in semi-batch emulsion polymerization. **W. Gerlinger**, O. Naeem, E. Jahns

3:00 Intermission.

3:30 POLY 365. Z-mer lengths revisited with a modern phase behavior model. **S.G. Arturo**, G. Dombrowski, R. Even, W. Gao, J.M. Martinez, B. McCulloch, T. Zhang

3:50 POLY 366. In situ spectroscopic studies of highly transparent PSMA-PTFEMA diblock copolymer dispersions in non-polar media. **E. Cornel**, S.P. Armes

4:20 POLY 367. Multiblock copolymer nanoparticles synthesized via RAFT aqueous emulsion polymerization using a high-throughput robot. **A. Cockram**, N.S. Williams, M.W. Murray, S.N. Emmett, S.P. Armes

Cellulose & Other Structural Biopolymers: Structure, Formation & Degradation: Anselme Payen Award Symposium in Honor of Junji Sugiyama
Sponsored by CELL, Cosponsored by BIOL, BIOT and POLY

Lignin: From Fundamentals to New Materials & Applications

Lignin Valorization in Biorefineries

Sponsored by CELL, Cosponsored by ENVR and POLY

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center Hall D

Adaptive Nanogels
Cosponsored by COLL
A. Fernandez-Nieves, T. Hoare, L.A. Lyon, W. Richtering, D. Suzuki, *Organizers*

6:00–8:00

POLY 368. Synthesis of micron-sized poly(*N*-Vinylcaprolactam) microgels by temperature-ramp polymerization. **A. Ksiazkiewicz**, A. Pich

POLY 369. Microfluidically produced microgels with biomedical applications. **A.J. Kuehne**, L. Elling, L. De Laporte, G. Sellge, A. Jans, L. Guerzoni

POLY 370. Hollow charged microgels: Structural investigations by SANS. **S.K. Turnhoff**, A. Scotti, W. Richtering

POLY 371. Design and synthesis of rotaxane crosslinked polymeric microspheres. **S. Hirohsige**, T. Kureha, J. Sawada, D. Aoki, T. Takata, D. Suzuki

POLY 372. Interplay of spatially separated polymeric shells in doubly thermoresponsive microgels in presence and absence of an incompressible core. **M. Brugnoni**, A. Scotti, A. Rudov, A. Gelissen, A. Radulescu, I. Potemkin, W. Richtering

POLY 373. Bioorthogonal preparation of dPG-based nanogels using iEDDA inverse nanoprecipitation. **A. Oehrl**, R. Haag

POLY 374. Microgels decorated with 2-methoxyethyl acrylate as new building block for biomaterials. **A. Melle**, S. Moli, L. De Laporte, W. Richtering, A. Pich

POLY 375. Withdrawn

POLY 376. Directed immobilization of thermo-responsive functionalized microgels via DNA. **S. Eisold**, C. Molano Lopez, A. Tran, A. Oppermann, D. Wöll, D. Mayer, A. Pich, U. Simon

POLY 377. Distribution of ionizable groups in polyampholyte microgels controls interactions with captured proteins: From blockade and "levitation" to accelerated release. **W. Xu**, A. Pich, I. Potemkin, W. Richtering, A. Rudov, R. Schröder, I. Portnov

POLY 378. Synthesis of hydrogel/solid composite microgels by seeded emulsion polymerization in the presence of polyelectrolytes microgels. **T. Watanabe**, S. Chihong, K. Murata, T. Kureha, D. Suzuki

POLY 379. Monte Carlo simulations of weak polyelectrolyte nanogels: pH-dependence of conformation and ionization. **C. Hofzumahaus**, S. Schneider

POLY 380. Polyelectrolyte microgels oppose electrodeposition. **S. Schneider**, O. Mergel, F. Plamper

POLY 381. Fluorescence microscopy investigation of microgels at interfaces. **E. Siemes**, M. Faulde, A. Jupke, D. Woell

POLY 382. Real-time adsorption behavior of hydrogel microspheres onto solid/liquid interface. **S. Matsui**, T. Uchihashi, D. Suzuki

POLY 383. Investigation of highly charged microgels at flat liquid-liquid interfaces. **M.M. Schmidt**, W. Richtering

POLY 384. Dynamics of large poly(*N*-isopropyl acrylamide)-based hydogel microspheres at the air/water interface. **H. Minato**, T. Watanabe, D. Suzuki

POLY 385. Probing the internal heterogeneity of responsive microgels adsorbed to an interface by sharp tip SFM. **M. Schulte**, A. Scotti, A. Gelissen, M. Ahmed, W. Richtering

POLY 386. Thermo-responsive microgels at interfaces: Correlation between microgel softness and monolayer properties. **S. Bochenek**, A. Scotti, W. Richtering

POLY 387. Versatile nanoreactors based on temperature-responsive microgels. **D. Kleinschmidt**

POLY 388. Withdrawn

POLY 389. Molecular separation by stimuli-responsive hydrogel microspheres. **T. Kureha**, K. Hosho, D. Suzuki

POLY 390. Withdrawn

POLY 391. Dynamic investigations of the cononsolvency of poly-N-isopropylacrylamide microgels. **K. Nothdurft**, T. Brands, A. Bardow, W. Richtering

‡*Cooperative Cosponsorship*

POLY 392. Rheology of dense suspensions of temperature-responsive microgel mixtures. **S. Minami**, T. Watanabe, D. Suzuki, K. Urayama

Section A
Ernest N. Morial Convention Center
Hall D

Excellence in Graduate Polymer Research
Cosponsored by PRES, PROF, SOCED and YCC
H. Cheng, C. Ellison, C.J. Landry-Coltrain, T.E. Long, *Organizers*

6:00–8:00

POLY 393. Investigation of mechanochemical reactivity of 1,2-oxazines. **V. Kensy**, D.C. Church, A.J. Boydston

POLY 394. Synthesis and melt self-assembly of tapered bottlebrush copolymers. **L. Jiang**, D. Nykypanchuk, A. Ribbe, J. Rzayev

POLY 395. Synthesis of hydrolysis-resistant polyisobutylene-based polyurethanes. **J. Kantor**, E. Collister, J.E. Puskas, M.P. Mallamaci, V.C. Comes

POLY 396. Investigation of PVDF block copolymer architecture and their interface properties. **V. Vasu**

POLY 397. Synthesis of [FeFe]-hydrogenase mimetic metallopolymers via ATRP for robust and O_2 resistant H_2-evolution catalysts. **M. Karayilan**, W.P. Brezinski, D.L. Lichtenberger, R.S. Glass, J. Pyun

POLY 398. Solvent free addition of allyl and vinyl monomers into polysulfides formed by inverse vulcanization. **C. Westerman**, C. Jenkins

POLY 399. Platinum(II) end-capped glycerol/adipic acid poly(ester)s as antitumor prodrugs. **U.G. Huynh**, B.A. Howell

POLY 400. Aqueous-processed, high-capacity electrodes for membrane capacitive deionization (MCDI). **A. Jain**, J. Kim, Q. Li, R. Verduzco

POLY 401. Sulfonated terpolymers as proton exchange membranes for fuel cells: effect of aliphatic groups. **A. Jinju**, K. Miyatake

POLY 402. Recent advances in achieving nanofiller miscibility with polyolefin matrices. **J. Pribyl**, M. Bell, K.B. Wagener, B.C. Benicewicz

POLY 403. Enhanced conjugated polymer nanofiber network formation by synergistic effect of solution shearing and dielectric layer modification. **Z. Yuan**, S. Thomas, C. Buckley, G. Zhang, J.E. Bredas, E. Reichmanis

Section A
Ernest N. Morial Convention Center
Hall D

General Topics: New Synthesis & Characterization of Polymers

D. Garcia, *Organizer*

6:00–8:00

POLY 404. Thermal analysis of poly(methylmethacrylate) (PMMA)-graphene oxide(GO) composites. **I.J.A Don**, F.D. Blum

POLY 405. Thermal analysis of poly(ethyl methacrylate) adsorbed on silica. **R. Azarfam**, U.N. Arua, F.D. Blum

POLY 406. Elucidating end group effects on the degradation of linear polyethylene glycol using matrix assisted laser desorption ionization time of flight (MALDI-TOF) mass spectrometry. **M.E. Payne**, S.M. Grayson

POLY 407. Effect of equivalent weight on the dynamic mechanical relaxations of perfluorosulfonic acid membranes. **M. Novy**, R.B. Moore

POLY 408. Comparative study of dielectric relaxation and electrical conductivity behavior correlated to hydrogen bonding organization between Bis-MPA based hyperbranched polymer and dendrimer. **B. Chen**, J.A. Giesen, M.K. Hassan, S.M. Grayson, S.I. Nazarenko

POLY 409. Responsive DNA-like polymers via the ring opening polymerization of nucleobase appended thiolactones. **S. Mavila**, B. Worrell, T. Goldman, C. Wang, B.D. Fairbanks, D.W. Domaille, S. Pattanayak, M.K. McBride, C. Bowman

POLY 410. Guanidinium-functionalized polymer carriers enable RNAi in resistant insect pests. **K.H. Parsons**, M.H. Mondal, C.L. McCormick, A.S. Flynt

POLY 411. Dendrimer-based probes for investigating size restrictions of transdermal permeability. **K. Kosakowska**, S.L. Kurtz, L.B. Lawson, S.M. Grayson

POLY 412. Meta-linked cationic poly(phenylene ethynylene) conjugated polyelectrolyte featuring a chiral side group: Helical folding and phosphates binding. **Z. Li**, K.S. Schanze

POLY 413. Template-directed synthesis of well-defined polysaccharides. **A. Delawder**, A.F. Greene, X. Li, J. Barnes

POLY 414. RAFT synthesis of ABA-BAB type PS-PVBC triblock copolymers for polyelectrolyte materials. **O. Ozcalik**, M.L. Anthamatten

POLY 415. Hyperbranched bisphosphonate-functional polymers via RAFT self-condensing vinyl polymerization and post-polymerization functionalization. **P.R. Calvo**, K.B. Wagener, B.S. Sumerlin

POLY 416. Thermoresponsive hyperbranched block copolymers via RAFT self-condensing vinyl polymerization. **P.R. Calvo**, K.B. Wagener, B.S. Sumerlin

POLY 417. Effect of pendant groups on fabrication of poly(norbornene imide) single-chain nanoparticles. **R. Chen**, S. Benware, J.J. Lessard, J. Cole, E.B. Berda

POLY 418. Handles for controlled architecture and functionality in single-chain nanoparticles: Cross-linking by intrachain ATRP. **E.R. Bright**, C. Willis, C. Leo, N. Shipley, C.J. LaSalle, A. Hanlon, E.B. Berda

POLY 419. Hydrogenated polyisoprene-*g*-silica nanoparticles in polyolefin nanocomposites. **M.M. Mohammadkhani**, Z.M. Abbas, B.C. Benicewicz

POLY 420. Synthesizing single-chain nanoparticles: Bio-inspired functionality *via* isocyanide-based multicomponent reaction chemistry. **E. Reville**, J. Cole, J.J. Lessard, K. Rodriguez, A. Hanlon, J.P. Mancinelli, E.B. Berda

POLY 421. Designing free-radical redox photoinitiators for practical dark curing. **K. Kim**, J. Sinha, C. Musgrave, J.W. Stansbury

POLY 422. Polymeric chromophore-catalyst assembly for the photocatalytic CO_2 reduction. **Y. Zhao**, S. Kim, Y. Eom, G. Leem, K.S. Schanze

POLY 423. Organocatalytic synthesis of poly(thionolactone)s: New materials abilities from sulfur-containing polylactones. **P. Datta**, I. Kalana, R. Hewawasam, M.K. Kiesewetter

POLY 424. Anion conductive polymers consisting of perfluoroalkylene, fluorenyl, and pendant ammonium groups. **N. Yokota**, H. Ono, J. Miyake, K. Miyatake

POLY 425. Photo controlled two-stage reactive polymer construction and application. **X. Zhang**, S. Huang, W. Xi, K. Long, C. Bowman

POLY 426. A modular approach to semi-fluorinated aromatic ether polymers via step-growth polymerization of fluoroalkenes. **K. Shelar**, K. Mukeba, A. Sygula, D.W. Smith

POLY 427. Xerogel-sequestered transition metal catalysts: A new generation of marine antifouling materials. **C.A. Damon**, M.R. Detty

POLY 428. Self-initiated functionalization of waste tire rubber networks and new composite applications. **E. Caldona**, T. Rosenmayer, D.W. Smith

POLY 429. Structure/property/processing relationships in POSS-modified high temperature thermoplastic composites. **M.B. Woellner**, **R. Shankar**, A.F. Stewart, K.T. Posey, J.D. Lichtenhan, S.E. Morgan

POLY 430. Polyolefins as tools for multiwalled carbon nanotubes solubilization. **P.K. Manyam**

POLY 431. Modification of sulfonated syndiotactic polystyrene aerogels through ionic interactions. **X. Li**

POLY 432. Ultrahigh heat-resistance polybenzimidazole/polyamide from *Streptomyces*-derived biomonomers. **A. Nag**, T. Kaneko

POLY 433. Saturated *N*-heterocyclic cationic polymers: Synthesis and stability. **R. Sun**, Y.A. Elabd

POLY 434. Formation of poly(norbornene) thioacetate and deprotection into polythiols. **C. Barrios**, C. Jenkins

POLY 435. Ring opening polymerization of lactones by a neodymium coordination catalyst. **R. Kularatne**, C. Bulumulla, H. Nguyen, M.C. Stefan

POLY 436. Synthesis of ionically crosslinked polyelectrolytes by homopolymerization of an ion-pair comonomer. **C. Li**

Section A
Ernest N. Morial Convention Center
Hall D

Integrating Polymer Science in the Curriculum
Cosponsored by CHED and PMSE
K.R. Carter, K.A. Cavicchi, S.E. Morgan, *Organizers*

6:00–8:00

POLY 437. Integrating polymer chemistry in the Undergraduate Chemistry Department at Hofstra University. **R.P. D'Amelia**

POLY 438. Microwave and neat synthesis of 7-oxanorbornene derivatives for organic chemistry teaching lab: A comparison study. J. Bazemore, M. Kelly, L. Phan, **B.P. Quillian**, **S. Zingales**

POLY 439. Towards open and interactive sharing of polymer membrane gas separation data. **J.E. Bara**, **V.F. Scalfani**, **W.R. Raney**

POLY 440. Teaching a polymer chemistry course at a primarily undergraduate institution. **J.C. Furgal**

Section A
Ernest N. Morial Convention Center
Hall D

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Cosponsored by BIOT, MEDI and PMSE
M.B. Baker, R. Kieltyka, F.A. Leibfarth, J.B. Matson, *Organizers*

6:00–8:00

POLY 441. Polyion complex micelle incorporating TiO_2 nanoparticles for effective sonodynamic therapy. **S. Yamamoto**, K. Furukawa, M. Ono, E. Yuba, A. Harada, K. Kono

POLY 442. Mannose residue-introduced pH-sensitive curdlan-modified liposome for antigen presenting cell-specific antigen delivery system. **Y. Fukaya**, E. Yuba, A. Harada, K. Kono

POLY 443. A gene delivery approach using zwitterion-modified dendrimer-entrapped gold nanoparticles for inhibition of cancer cell metastasis. **Z. Xiong**, C. Alves, A. Li, F. Chen, J. Liu, M. Shen, H. Tomas, X. Shi

POLY 444. Liver-specific DDS using liposomes modified with sugar moiety-introduced dendron lipids and pH-responsive polymer-lipids. **Y. Hayashi**, E. Yuba, A. Harada, K. Kono

POLY 445. Cationic poly(peptidophosphoesters) and poly(peptidosaccharides) for antimicrobial therapy. D. Pranantyo, M. Chan Park, K. Neoh, **E. Kang**

POLY 446. Development of multifunctional nanohybrid: antibody-conjugated gold nanorods stabilized by functional dendrimer for targeted photothermal therapy and imaging. **H. Setiawan**, E. Yuba, A. Harada, I. Aoki, K. Kono

POLY 447. Development of hyaluronic acid derivative-modified liposomes as dendritic cell-specific antigen delivery carriers. **M. Miyazaki**, E. Yuba, H. Hayashi, A. Harada, K. Kono

POLY 448. Multifunctional nanohybrids

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composed of functional dendrimer and gold nanorod for photothermal-chemotherapy. **T. Hashimoto**, E. Yuba, A. Harada, K. Kono

POLY 449. Hydrogels based on peg and chitosan-reduced graphene oxide for volumetric muscle loss treatment. **J.F. Petry**, D. Gamba

POLY 450. Polysulfides... a 'break-through' for osteoporosis? **F. El Mohtadi**

POLY 451. Synthesis and characterization of chitosan derivatives for high performance gene delivery. **Q. Wyatt**

POLY 452. Polyglycidol-based hydrogels for applications in regenerative medicine. **B. Loftin**, E. Harth

POLY 453. Terpene-based polymers by step-growth polymerization: Renewable monomers and polymers for biomedical applicaitons. **D. O'Brien**, S.M. Howdle, C. Alexander, R.A. Stockman

POLY 454. Withdrawn

POLY 455. Bioinspired polymer composites for antifouling surface coatings. **I.S. Kurtz**, A. Sathyan, T. Emrick, J.D. Schiffman

POLY 456. Electroactive hydrogels for biomedical applications. **Z. Shi**, G. Yang

POLY 457. Surface plasmon resonance study of interaction between membrane protective block copolymers and supported lipid bilayer. **M. Kim**, M. Vala, S. Oh, F. Bates, B.J. Hackel

POLY 458. Controllable glucose-based bioadhesive through strain-promoted azide-alkyne cycloaddition (SPAAC). **I. Pramudya**, H. Chung

POLY 459. Role of transporter-cargo binding in polymer mediated intracellular protein delivery. **N.D. Posey**, C. Hango, G.N. Tew

POLY 460. Aspect ratio-controllable polyplexes prepared from poly(L-lysine) terminally bearing multi-arm PEG. **A. Harada**, E. Yuba, K. Kono

POLY 461. Rigid, fibrous-structured protein showed superior cell-penetrating activity. **K. Sano**, N. Nakayama, S. Takagaki, T. Takaoka, E. Ota

POLY 462. Conjugated polymers for RNA interference in human primary bronchial cells. P. Manandhar, M. Ahmed, **J. Moon**

POLY 463. Amphiphilic block copolymers, hydrogels, and micelles for the controlled release of HNO. **C. Lee**, D. Church, A.J. Boydston

POLY 464. Construction of core-shell tecto dendrimers based on supramolecular host-guest assembly for enhanced gene delivery. F. Chen, L. Kong, L. Wang, Y. Fan, M. Shen, **X. Shi**

POLY 465. Polymeric mimetics of antimicrobial peptides as anticancer agents. **F. Gao**, J. Piao, L. Hui, Y. Wang, L. Yang

POLY 466. Withdrawn

POLY 467. Radical copolymerization of vinyl ethers and cyclic ketene acetals as a versatile platform to design functional polyesters. **Y. Guillaneuf**

POLY 468. Variable charge density in siRNA-containing block ionomer complexes: Optimizing complex binding strength, stability, and gene suppression. **K.H. Parsons**, A.S. Flynt, C.L. McCormick

Section A
New Orleans Marriott Canal Street
Studio 6

International Symposium on Biorelated Polymers: Renewable Materials
Cosponsored by PMSE
E.W. Cochran, E.C. Hagberg, R.T. Mathers, A. Watts, *Organizers*

6:00–8:00

POLY 469. Washed cottonseed meal-based products as bio-based wood adhesives for non-structural interior applications. **Z. He**, H. Cheng

POLY 470. Preparation of anisotropic physical hydrogels of cyanobacterial super-polysaccharides. **M. Okajima**, T. Kaneko

POLY 471. Developing sustainable acrylates for 3D printing. **R. Goncalves**, R. Ding, T.M. Reineke

POLY 472. Sustainable and degradable epoxy resins containing multifunctional biobased components. **M. Shen**, G. Yang, R. Almallahi, Z. Rizvi, E. Gonzalez, T. Hendrix-Doucette, M.L. Robertson

POLY 473. Therapeutic electrospun natural polymer based fiber scaffolds for biomedical applications. K. Penton, W. Weeks, A. Wilson, Z. Kinler, V.F. Baker, T. Brown, S. Salter, **S.K. Hamilton**

Section A
Ernest N. Morial Convention Center
Hall D

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
Cosponsored by PHYS and PMSE
A. Mariani, J.A. Pojman, A. Taylor, *Organizers*

6:00–8:00

POLY 474. Withdrawn

POLY 475. Low-temperature frontal polymerization of acrylate-based composites for use in bone repair. **S. Bynum**, C. Morejon-Garcia, M.P. Tullier, J.A. Pojman

POLY 476. Time-lapse materials: Using the enzymatic hydrolysis of urea in polymerization. **D. McKenzie**, J.A. Pojman

POLY 477. Mechanistic insight into alkyl phosphite inhibited frontal ring-opening metathesis polymerization. **G. Rudebusch**, J. Moore

POLY 478. Preparation of acrylic acid-*graft*-carboxymethyl cellulose superabsorbent hydrogels by frontal polymerization. **S. Li**

POLY 479. Frontal polymerization of deep eutectic solvents composed of acrylic and methacrylic acids. **K.F. Fazende**, J.A. Pojman

POLY 480. Radical-induced cationic frontal polymerization using divinyl ethers. **B. Thompson**, J.A. Pojman

POLY 481. Chemical oscillating particles through encapsulation of the urea-urease reaction. **A. Mai**

Section A
Ernest N. Morial Convention Center
Hall D

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*

6:00–8:00

POLY 482. Cyclic versus acyclic acetal-based monomers: Using monomer design and thiol-ene photopolymerization to tailor network architecture and degradation profiles. **W.D. Walker**, D.N. Amato, D.V. Amato, W. Martin, S. Swilley, M. Sandoz, M. Vekasy, D.L. Patton

POLY 483. Utility of photolabile protecting groups in amine functionalized polymers. **W.T. De Alwis**, P. Kurek, D. Konkolewicz

POLY 484. Layered polymer networks with dual-cure mechanisms based on multi-functional benzoxazines. **J. Weigand**, C. Miller, J.S. Wiggins

POLY 485. Application of core modified phenoxazine photoredox catalysts in organocatalyzed atom-transfer radical polymerization. **B. McCarthy**

POLY 486. Photoresponsive surface wrinkling in polymer brush thin films. **C. Reese**, P. Logan, B. Thompson, D.L. Patton

POLY 487. Excited state dynamics and exciton diffusion in platinum-acetylide polymers. **R. He**, R. Acharya, K.S. Schanze

POLY 488. Synthesis of acetal-based multifunctional thiols as building blocks for degradable poly(thioether acetal) thermosets via thiol-ene photopolymerization. **M. Vekasy**, D.N. Amato, D.V. Amato, C.A. Sarantes, W. Walker, D.L. Patton

POLY 489. Synthesis of photo-responsive optically active conjugated polymers and photo-reaction field. **M. Otaki**, H. Goto

Section A
Ernest N. Morial Convention Center
Hall D

Polymer Applications & Characterization in Medical Device & Pharmaceutical Industries
Cosponsored by PMSE
Financially supported by Pfizer
X.M. Liu, J. Slager, *Organizers*

6:00–8:00

POLY 490. Effect of branching (star architecture) on poly(d,l-lactide) (PDLLA) degradation and drug delivery. **R. d'Arcy**

POLY 491. Development of antimicrobial-loaded polyurethane films for drug-eluting catheters. **M. Barde**, **M. Davis**, H. Mendis, L. De La Fuente, M. Auad

POLY 492. Novel bacterial anti-adhesion films with polymers derived from natural products. **K. Long**, J. Sinha, C. Bowman

POLY 493. Design of synergistic drug crystallization inhibitors via olefin cross-metathesis of hydrophilic cellulose ethers and bile acid derivatives. **D. Novo**, K.J. Edgar, L. Taylor, L.I. Mosquera-Giraldo

Section A
Ernest N. Morial Convention Center
Hall D

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COMP and PMSE
J. Bohling, W. Gao, D.N. Haase, J. Tsavalas, W. Wu, *Organizers*

6:00–8:00

POLY 494. Characterization of acrylic alkali soluble polymer dispersions by asymmetrical flow field-flow fractionation. **G.P. Abramo**, W. Gao, L. Rhodes, J. Park

POLY 495. High-performance polymers for industrial applications. **D.N. Haase**, Z. Fu, A. Bacho, A. Pratt

POLY 496. Chemistry which enabled coatings with polymer pigment self-assembly to become a commercial reality. **J. Bohling**, K. Beshah, M. Clark, A.M. Maurice, W. Gao, S. Brownell, J.R. Reffner

POLY 497. Fundamental understanding of acidic monomer incorporation in acrylates emulsion polymerization. **W. Gao**, **P. Luo**, A.M. Maurice, T. Zhang, W. Young, C. Johann, S. Elsenberg

Section A
Ernest N. Morial Convention Center
Hall D

Polymer Networks: Soft Gels to Stiff Networks
Cosponsored by PHYS, PMSE and SOCED
E. Chan, S. Kundu, R.B. Moore, *Organizers*

6:00–8:00

POLY 498. Analysis of segmental dynamics for rigid crosslinked system using low field NMR. W. Zhao, J. Patel, X. Tao, **S.L. Hsu**

POLY 499. Thermally responsive and conductive PNIPAM hydrogel spheres. **D. Varghese**, D.H. Adamson

POLY 500. How do cross-linking kinetics relate to rheological property evolution in thermoset coatings? **J. Tilly**, D. Inglefield, R.J. Spontak, S. Khan

POLY 501. Controlled storage and release of elastic energy in crosslinked polymer microparticles. **L. Cox**, W. Li, J. Leng, J. Xiao, **Y. Ding**

POLY 502. Elastic multi-functional poly (ionic liquids) membrane. **B. Li**, P. Cao, S. Zhao, K. Xing, J. Hingu, A.P. Sokolov, T. Saito

POLY 503. Reprocessable cross-linked polyurethanes. **D.J. Fortman**, J. Brutman, R.L. Snyder, M.A. Hillmyer, W. Dichtel

POLY 504. Influence of trifluoromethyl substituents on optical properties of polyimide aerogels. **S.L. Vivod**, M. Meador, C.R. Pugh

POLY 505. Thiol-ene networks containing perfluorinated n-alkanes: Effect of n-alkane length on free-volume and gas permeation. **V. Vasagar**, R. Ramakrishnan, J. Goetz, B.M. Ameduri,

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S.I. Nazarenko

POLY 506. Development of thermally reversible polyimide gels for coating carbon nanotube wires. **R.P. Viggiano**, J.J. Maldonado, B.N. Nguyen, H.N. Guo, L.S. McCorkle, T. Williams, M. Meador

POLY 507. Nanomechanics of thin poly(methacrylic acid) multilayer hydrogels probed by AFM. **K.A. Stockmal**, V.A. Kozlovskaya, E.P. Kharlampieva, S.E. Morgan

POLY 508. Actuation of viologen-based soft materials using a photoredox mechanism. **K. Liles**, A.F. Greene, M. Danielson, A. Wellen, N.D. Colley, J. Fisher, J.C. Barnes

POLY 509. Redox-to-donor-acceptor interconversion of supramolecular hydrogels. **A.F. Greene**, M.K. Danielson, A. Wellen, A. Natraj, N.D. Colley, J.C. Barnes

POLY 510. Synthesis and characterization of composite hydrogel networks for use in high performance concrete. **T.L. Thornell**, M.J. Krafcik, K.A. Erk

POLY 511. Advances in polyester vitrimer design. **J.L. Self**, M. Sanchez Zayas, A. Abdilla, J. Read De Alaniz, C. Bates

POLY 512. Ghost particles: Effect of constrained space on glassy polymer network formation and mechanics. **T. Palmer**, J. Winetrout, J.S. Wiggins

POLY 513. Porous LAdder-polymer networks (PLANs). **S. Che**, L. Fang

POLY 514. Bringing furan/maleimide Diels-Alder HA hydrogel chemistry to physiological conditions, for biomedical applications. **V. Delplace**, A. Amin, M.S. Shoichet

Section A
Ernest N. Morial Convention Center
Hall D

Polymer Optoelectronics

J.D. Azoulay, X. Gu, Y.C. Simon, *Organizers*

6:00–8:00

POLY 515. Correlating molecular structure with the optoelectronic properties of tailored oxoverdazyl radical species. **V. Agarkar**, B.W. Boudouris

POLY 516. Structure-mechanical property of stretchable organic ultra-thin film for electronic applications. B. Appleby, **S. Zhang**, X. Gu

POLY 517. Simple and rapid functionalization of conjugated polymers via thiol-ene "click" chemistry. **J. Tropp**, D.V. Amato, D.L. Patton, J. Azoulay

POLY 518. Donor–acceptor polymers with tunable infrared photoresponse. **L. Huang**, A.E. London, T. Ng, J. Azoulay

POLY 519. Structure-function property relationships of narrow bandgap donor-acceptor polymers containing selenium. **N. Eedugurala**, J.D. Azoulay

POLY 520. Interface engineering of air-processed inverted OPV devices via sol-gel processed vanadium oxide hole-extraction layer. **A.R. Benasco**, **J. Richardson**, L. Moore

POLY 521. Incorporation of DNA aptamers into conjugated polymer-based optical sensors. **J.O. Peter**

Section A
Ernest N. Morial Convention Center
Hall D

Structure & Dynamics of Materials via NMR Spectroscopy

Financially supported by Exxon, NMR Service, Rototec-Spintec

H. Cheng, *Organizer*

6:00–8:00

POLY 522. Enzyme-catalyzed "click" Michael addition between fluorescein monoacrylate and thiol-functionalized polyethers. **G. Shrikhande**, S. Sen, P. Mulay, J.E. Puskas

POLY 523. Synthesis of thiol-functionalized tetraethylene glycol and poly(ethylene glycol)s via enzyme-catalyzed transesterification. **P. Mulay**, S. Sen, J.E. Puskas

POLY 524. Structural studies of polydisulfide macrocycles by 2D gHMBC NMR. **S. Sen**, V. Dudipala, J.E. Puskas

POLY 525. Chemical degradation of model sulfonated polyphenylene proton exchange membranes. **C. Miller**, E.G. Sorte, T.M. Alam

POLY 526. Miscibility analysis of polymer based ultrafiltration membranes through two dimensional WIdeline SEparation solid state NMR spectroscopy. **K. Dizon**, J.D. Oliver, G. Johnston-Hall, R. Wuhrer, P. Castignolles, M. Gaborieau

POLY 527. Understanding polymer dynamics in perfluorosulfonic acid membranes *via* solid-state NMR. **Z.B. Yan**, A.P. Young, G.R. Goward

POLY 528. ^{19}F spin diffusion and X-ray scattering analysis of fluoropolymers. **J. Vaughn**, J. Hammons, H. Mason

POLY 529. NMR investigations of dynamics in the different phases of semicrystalline polymers. **M. Schaefer**, R. Kurz, A. Seidlitz, M. Schulz, T. Thurn-Albrecht, K. Saalwaechter

POLY 530. Characterisation of industrial adhesives with (solid-state) NMR spectroscopy. K. Bhullar, J.J. Thevarajah, A. Rebmann, S. Cheevers, R. Wuhrer, P. Castignolles, **M. Gaborieau**

POLY 531. Detection of nanoscale phase separation in nanoparticles with mixed ligand shells. **B.I. Guzman Juarez**, K. Kim, A. Abdelaal, S. Allie, V. Toader, L.G. Reven

POLY 532. ^{2}H-NMR, FTIR, and DSC: The structure and dynamics of poly(styrene-r-methyl methacrylate-d$_3$) on silica. **U.N. Arua**, M. Maddumaarachchi, F.D. Blum

POLY 533. Effect of water on the structure and dynamics of [3-^{13}C] Ser, [3-^{13}C] Tyr and [3-^{13}C] Ala-*Bombyx mori* silk fibroin studied with ^{13}C solid-state NMR. **A. Nishimura**, H. Matsuda, Y. Tasei, T. Asakura

POLY 534. Chain conformation, packing, and folding structures of poly(L-lactic acid) in glassy state as studied by ^{13}C solid-state NMR and selective isotope labeling. **S. Yuan**, S. Wang, T. Miyoshi

POLY 535. Crystal structure of poly(lactic acid) stereocomplex as studied by ^{13}C-^{13}C double quantum NMR. **W. Zhou**, S. Wang, S. Yuan, T. Miyoshi

POLY 536. Effect of stereoregularity on local dynamics of hydrogenated polynorbornenes as studied by solid-state NMR. **Y. Makita**, Y. Nakama, S. Hayano, H. Kurosu, T. Miyoshi

Section A
Ernest N. Morial Convention Center
Hall D

Undergraduate Research in Polymer Science
Cosponsored by CHED and PMSE
H. Broadhead, S.E. Morgan, S.I. Nazarenko, *Organizers*

6:00–8:00

POLY 537. Imidazolium-containing thiol-ene poly(ionic liquid) membrane networks: Conductive and gas separation properties. **A.F. Bratton**, H.B. Fannin, K.M. Miller

POLY 538. Trithiocarbonate disulfides as chain transfer agents. **T. Ruiz Velasco**, D.K. Schneiderman, A. Way, S.J. Rowan

POLY 539. Methylene blue doped polymer films for anaphylaxis treatment: Film morphology and drug dispersal. **H. Fischer**, R.M. Van Horn

POLY 540. Design, synthesis and characterization of polyimides containing pyridine/pyridinium linkages in their backbones. **V. Levine**, M.E. Verde, G.P. Dennis, D. Mecerreyes, J.E. Bara

POLY 541. Synthesis and characterization of a DFDPP-CPDT polymer with ethynyl spacers by means of a Sonogashira coupling. **H.P. Masching**, **C. Benson**, J.L. Duffy-Matzner

POLY 542. Synthesis towards sequence-controlled polypeptides. **C. Morejon-Garcia**, R.A. Letteri, T. Nguyen, Y. Tsao, X. He, K.L. Wooley

POLY 543. Interface optimization of nanoaluminum urethane composite energetic foams. **C. Baxter**, J. Bencomo, J. McCollum, S.T. Iacono

POLY 544. Epoxy based liquid crystal elastomers for shape memory materials. S.T. Iacono, N. Godman, T.J. White, J.M. McCracken, **C. Baxter**

POLY 545. Mechanical testing for stretchable organic thin film for electronic applications. **B. Appleby**, S. Zhang, X. Gu

POLY 546. Dynamic, responsive DNA-like polymers. **T. Goldman**, B.T. Worrell, S. Mavila, C. Bowman

POLY 547. Dynamic thiol-Michael bonds in poly(ionic liquid) polyester networks. **S.P. Daymon**, K.M. Miller

POLY 548. Anionic ring-opening polymerization of activated azetidines. **E.A. Rowe**, L. Reisman, P. Rupar

POLY 549. Fluorinated polyfulvenes for low band gap optical applications. **C. Bestler**, A. Peloquin, G.J. Balaich, **S.T. Iacono**

POLY 550. Determination of equilibrium water content in bioinspired glycopolymer hydrogel networks. **H.E. George**, B.S. Upadhyay, K.A. Stockmal, S.E. Morgan

POLY 551. Synthesis of anionic acrylamide-based polymers for determination of structure/binding interactions with food-based proteins. **A.N. Davis**, B.E. Payne, A.N. Bristol, S.E. Morgan

POLY 552. Monitoring the effect of crosslink density and amphipathic balance on viscoelastic property evolution in glycopolymer hydrogels using rheology. **B.S. Upadhyay**, A.L. Fogel, S.E. Morgan

POLY 553. Synthesis of *p*-xylene-diisocyanide and polymerization to form poly(2,4-pyrrole-alt-*p*-phenylene). **J.P. Mancinelli**, J. Cole, E.B. Berda

POLY 554. Withdrawn

POLY 555. pH responsive sulfonamide-based polysoaps via RAFT copolymerization for oil remediation and recovery. **K. Stevens**, P.D. Pickett, C.L. McCormick

POLY 556. Highly conductive composites of intrinsically conductive conjugated polymers and carbon nanotubes. **G. LeCroy**, L. Huang, J. Azoulay

POLY 557. Electrospun silk fibroin for use as biomechanical actuators. **S. Maxwell**, S. Severt, J. Bontrager, A. Murphy

POLY 558. Responsive "polysoaps" via RAFT copolymerization to serve as therapeutic drug delivery vehicles. **M.A. Dearborn**, P.D. Pickett, C.L. McCormick

POLY 559. Withdrawn

POLY 560. *Endo* vs. *Exo*: Temperature tunnable functional building blocks for highly efficient polymer modification. **S. Nguyen**, A. St. Amant, E. Discekici, J. Read De Alaniz, C.J. Hawker

POLY 561. Block crystallization mechanisms of PEO-b-PCL as a function of weight fraction and isothermal crystallization temperature. **C.W. Tower**, R.M. Van Horn

POLY 562. Plasma treatment of rough polymer surfaces to achieve increased diffuse reflectance. **K. Ardrey**, A. Erickson, P. Defino, C.S. Coughlin, H. Chintakunta, C. Drake

POLY 563. Cohesion in layered polymer networks prepared by stereolithography. **C. Croshaw**, J. Weigand

POLY 564. Phosphazene-base promoted ring-opening polymerization of 1,2-butylene oxide and ethoxyethyl glycidyl ether initiated by secondary amides. **A. Shishlov**, P. Guégan, N. Illy

POLY 565. Zinc oxide nanoparticle composites from keratin, cellulose and chitosan: Antimicrobial properties and synthesis. **S. Sterling**, J. Nyakuchena, E. Munson, C.D. Tran

POLY 566. Withdrawn

POLY 567. Spheres from flat polymer sheets using only light. **D. Mong'are**, A. Hubbard, J. Genzer, M.D. Dickey

POLY 568. Synthesis of two fluorescent conjugated polymers with urea receptors

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as chemical sensors to detect fluoride ions. **A. Bah**, W. Wu, W.E. Bernier, W.E. Jones

POLY 569. Solvent effects of melting behavior of diblock copolymers of equal weight fractions. **D. O'Connor**

POLY 570. Synthesis of single-chain nanoparticles under various ATRC reaction conditions. **C. Leo**, E.R. Bright, C. Willis, A. Hanlon, E.B. Berda

POLY 571. Investigating the relationship between MOF modification and polymer-filler compatibility in thiol-ene based mixed matrix membranes. **G.A. Rodriguez**, J.M. Schekman, Y.C. Simon

POLY 572. Fabrication of polymer nanoparticles via intrachain ring-opening metathesis polymerizations (ROMP). **S. Benware**, R. Chen, J. Cole, E.B. Berda

POLY 573. Microwave assisted synthesis of polysuccinimide and polyaspartic acid for second semester organic chemistry students. N. Madrid, S. Moyer, **B.P. Quillian**, N. Shank

POLY 574. Withdrawn

POLY 575. Poly(Aspartic Acid) PAA in the undergraduate curriculum: A multi-course approach. **M. Weiland**, N. Davis, S.E. Gray, W. Hiester

POLY 576. Thiol-ene photopolymerization as a facile route to pro-antimicrobial polymer networks with degradable acetals. **M. Sandoz**, D. Amato, D.V. Amato, L. Blancett, O. Mavrodi, W. Martin, S. Swilley, K. Parsons, G. Shearer, D. Mavrodi, D.L. Patton

POLY 577. Analyzing the nanomorphology of novel diblock copolymers for potential use as solid polymer electrolytes. **K.N. Gardiner**, D.A. Waldow

POLY 578. Common protocol for coupling reactions of multiple classes of polymeric radicals. E.S. Tillman, **M. Arce**

POLY 579. Investigating the co-assembly behavior of linear amphiphilic triblocks in the fabrication of polymer vesicles. **E. Ghimire**, F. O'Dowd, T. Chidanguro, Y.C. Simon

POLY 580. Synthesis of single-chain nanoparticles through photodimerization of anthracene via triplet-triplet annihilation upconversion. **A. Garrett**, D.R. Blank, T. Chidanguro, J.M. Schekman, X. Yu, N. Ayres, Y.C. Simon

POLY 581. Selective deprotection of cyclopentadiene as a platform for functional polymeric materials. **S. Shankel**, A. St. Amant, E. Discekici, S. Nguyen, J. Read De Alaniz, C.J. Hawker

POLY 582. Analyzing the effect of molecular weight on ionic conductivity of novel solid polymer electrolytes for use in lithium ion batteries. **J. Finney**, D.A. Waldow

POLY 583. Analyzing the surface chemistry of polymer microgels as a function of particle stiffness. **C.A. White**, G.G. Brim, M. Gaines

Joint PMSE-POLY Poster Session

Clay-Polymer Composites: Nanoclay & Other Natural Nanoparticles

Sponsored by PMSE, Cosponsored by POLY

Joint PMSE-POLY Poster Session

General Posters: New Concepts in Polymeric Materials

Sponsored by PMSE, Cosponsored by POLY

Joint PMSE-POLY Poster Session

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

Sponsored by PMSE, Cosponsored by POLY

WEDNESDAY MORNING

Section A
New Orleans Marriott Canal Street Studio 6

International Symposium on Biorelated Polymers: Renewable Materials

Functionalization & Modification of Renewable Feedstocks

Cosponsored by PMSE
A. Watts, *Organizer*
E.W. Cochran, E.C. Hagberg, R.T. Mathers, *Organizers, Presiding*

8:00 POLY 584. Obvious and non-obvious bioaromatics for polymerization. **S.A. Miller**, M. Rostagno, S. Shen, G. Short, O. Nsengiyumva, F. Diot-Néant

8:40 POLY 585. Lignin-based functional polymers. **H. Liu**, H. Chung

9:00 POLY 586. Novel synthetic routes to polysaccharide-based block copolymers. **J. Chen**, K.J. Edgar

9:20 POLY 587. Cellulose nanocrystals in 3D printing and aerogels: nanocomposite properties. **R.C. Advincula**

10:00 Intermission.

10:30 POLY 588. New bio-related materials based on cardanol. **H. Cheng**, A. Biswas, Z. Liu, C.R. Alves, R.F. Furtado

11:00 POLY 589. Development of new biopolymers from renewable building blocks derived from low-molecular weight hemicelluloses. **L. Puchot**, R. Dieden, D. Da Silva Perez, **Y. Habibi**

11:20 POLY 590. Effect of the *N*-based ligands in copper complexes for depolymerisation of lignin. **J. Dai**, K. Saito, A. Patti

11:40 POLY 591. Thermoplastics from lignin oligomers and syringic acid derivatives. **L. Longe**, G. Garnier, K. Saito

Section B
New Orleans Marriott Canal Street Studio 1

Polymer Optoelectronics

X. Gu, Y.C. Simon, *Organizers*
J.D. Azoulay, *Organizer, Presiding*

8:00 POLY 592. In-situ materials structure measurements for organic photovoltaics manufacturing. **D. DeLongchamp**

8:30 POLY 593. Withdrawn

8:50 POLY 594. PTB7-Th-*b*-PNDI fully conjugated donor-acceptor block copolymers for thermal stability of photovoltaic devices. **Y. Lee**, E. Gomez, Q. Wang

9:10 POLY 595. Synthesis and characterization of benzodithiophene-*S,S*-tetraoxide based donor-acceptor polymers as organic semiconductors. **S. Adhikari**, D. Kim, T.L. Nelson

9:30 POLY 596. Polymer-acceptor bulk heterojunction solar cells: Establishing relationships among polymer chemical structure, polymer packing, and polymer-acceptor mixing. **J.E. Bredas**

10:00 Intermission.

10:30 POLY 597. Morphology in organic photovoltaics: Importance of intimately mixed donor/acceptor domains. **M. Toney**

11:00 POLY 598. Detectivity of shortwave infrared organic photodiodes. Z. Wu, W. Yao, A. London, J. Azoulay, **T. Ng**

11:30 POLY 599. Ultrafast singlet exciton decay in push-pull polymers. **M. Sfeir**

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Rheology, Melts & Gases

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
H. Kaji, *Presiding*

8:00 POLY 600. Quiescent and flow-induced crystallization of polyolefins studied by a novel low-field RheoNMR combination. V. Räntzsch, M.B. Özen, K. Ratzsch, G. Guthausen, **M. Wilhelm**

8:25 POLY 601. Viscoelasticity and structures in chemically and physically dual-crosslinked hydrogels: Insights from rheology and proton multiple-quantum NMR spectroscopy. **R. Zhang**, X. Zou, P. Sun

8:50 POLY 602. Polymers in electric fields and under shear studied by NMR. **U. Scheler**

9:15 POLY 603. Field-cycling NMR as a tool of molecular rheology. **M. Hofmann**, B. Kresse, N. Fatkullin, F. Fujara, E. Rössler

9:40 Intermission.

9:55 POLY 604. Unlinked cyclic polymers and the non-equilibrium melt state of UHMWPE; rheological, crystallization and mechanical response. **S. Rastogi**

10:20 POLY 605. Intermolecular contribution to proton spin-relaxation in polymer melts: New perspectives for experimental study of polymer melt dynamics.. **N. Fatkullin**, A. Lozovoi, C. Mattea, S. Stapf, E. Rössler

10:45 POLY 606. Intermolecular contribution to proton spin-relaxation in polymer melts: New experimental evidence for entanglement dynamics–does reptation really exist? A. Lozovoi, N. Fatkullin, C. Mattea, **S. Stapf**

11:10 POLY 607. NMR observations of the gases in polymers. **H. Yoshimizu**

Section D
New Orleans Marriott Canal Street Studio 2

Polymer Networks: Soft Gels to Stiff Networks
Cosponsored by PHYS, PMSE and SOCED
S. Kundu, R.B. Moore, *Organizers*
E. Chan, *Organizer, Presiding*

8:00 POLY 608. Tough hydrogels for time-programmable shapeshifting. **S. Sheiko**

8:30 POLY 609. Creating tough and healable macroscale "double network" hydrogels. **D.R. King**, R. Takahashi, T. Okumura, T. Sun, J.P. Gong

9:00 POLY 610. Double network hydrogels with high stiffness and ultra-high strength. **M. Grunlan**, A. Means

9:20 POLY 611. Highly resilient two component networks. **G.N. Tew**

9:40 POLY 612. Functional polymers through subcomponent self-assembly. **J. Nitschke**

10:00 Intermission.

10:30 POLY 613. Swelling and mechanical characterization of poly(acrylic acid)-based hydrogel particles used as internal curing agents in cement. **K.A. Erk**, T.L. Thornell, M.J. Krafcik

11:00 POLY 614. Stimuli-responsive supramolecular polymer networks. **C. Weder**

11:20 POLY 615. Emulsion templated hydrogels: Superabsorbents, stimulus-responsive, double-crosslinking, and dual-response. T. Zhang, S. Kovačič, **M.S. Silverstein**

11:40 POLY 616. Development of visible-light responsive and mechanically enhanced UCST double network hydrogels. **Y. Xu**, O. Ghag, P. Sitterle, M. Reimann, P. Chatterjee, E. Nofen, Y. Yu, H. Jiang, L. Dai

Section E
New Orleans Marriott Canal Street Studio 10

Adaptive Nanogels
Cosponsored by COLL
T. Hoare, L.A. Lyon, W. Richtering, D. Suzuki, *Organizers*
A. Fernandez-Nieves, *Organizer, Presiding*
A. Walther, *Presiding*

8:00 POLY 617. Hierachical mechanics and assembly in hydrogels. **P.J. Yunker**

8:30 POLY 618. Soft responsive microgels at high densities. **P. Schurtenberger**

9:00 POLY 619. Hard and soft

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microgels: Are they different? **W. Richtering**

9:30 POLY 620. Packing and defect tolerance of ultra-low cross-linked microgel assemblies. **L.A. Lyon**, M. Islam, R. Nguyen

10:00 Intermission.

10:30 POLY 621. Angle-independent structural colored materials by black and white components. **Y. Takeoka**

11:00 POLY 622. Hard core – Soft shell microgels for reconfigurable colloidal crystal assemblies. **A.J. Kuehne**, J. Sprakel, D. Go

11:20 POLY 623. Phase behavior in polydisperse microgel suspensions controlled by spontaneous particle deswelling. **U. Gasser**, **A. Scotti**, E.S. Herman, L.A. Lyon, A. Fernandez-Nieves

11:40 POLY 624. pH and temperature dependent swelling studies of core-shell microgels prepared with ultralow crosslinked microgels. **M. Islam**, L.A. Lyon

Section F
New Orleans Marriott Canal Street Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*
M. Allegrezza, D. Konkolewicz, *Presiding*

8:00 POLY 625. Recent advancements in optoelectronic materials. **L.M. Campos**

8:30 POLY 626. Withdrawn

8:50 POLY 627. Interrelationships between molecular structure, hierarchical organization, and FMO energies in supramolecular heterojunctions. **A. Levine**, C. Kolodziej, W. Lin, M. Ahmed, C. Burda, A.B. Braunschweig

9:10 POLY 628. Design and synthesis of fluorescent conjugated polyelectrolytes as copper and fluoride sensors. **W. Wu**, A. Bah, W.E. Bernier, W.E. Jones

9:30 POLY 629. Everything under the sun/light in polymers. **Y.C. Simon**

10:00 Intermission.

10:30 POLY 630. Beyond binary: Optical data storage in a quaternary code. **E. Pentzer**, P. Wei, B. Li, A. de Leon

11:00 POLY 631. Pixelated polymers: Directed self assembly of liquid crystalline polymer networks. **T.J. White**, B.R. Donovan, N. Godman, A. Auguste, T. Guin

11:30 POLY 632. Using light to actuate and locally tune the properties of polymers. **M.D. Dickey**, J. Genzer, Y. Liu, R. Mays, D. Davis, R. Mailen

Section G
New Orleans Marriott Canal Street Beauregard

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
A.N. Bristol, A.K. Naskar, K. Uchimura, *Presiding*

8:00 POLY 633. Iterative exponential growth synthesis of perfect triazole-based polymers. **Y. Jiang**, M. Golder, H.V. Nguyen, P. Teichen, Y. Shibuya, Y. Wang, M. Zhong, J.C. Barnes, D. Ehrlich, A. Willard, J.A. Johnson

8:20 POLY 634. Molecular design of water-soluble polyimides controlling rigidity and side chains. **T. Kaneko**, S. Sakamoto, T. Kobayashi, S. Dwivedi

8:40 POLY 635. Structure-kinetic relationships for mono(μ-oxo)-dialuminum initiators for epoxide polymerization. **J. Imbrogno**, R.C. Ferrier, N.A. Lynd

9:00 POLY 636. Controlled 2D polymerizations and resultant single crystal covalent organic frameworks. **A.M. Evans**, N. Flanders, L. Parent, R.P. Bisbey, E. Vitaku, N.C. Gianneschi, W. Dichtel

9:20 POLY 637. Block-stereoblock copolymers of poly(β-caprolactone) and poly(lactic acid). **T. Rosen**, I. Goldberg, W. Navarra, V. Venditto, M. Kol

9:40 POLY 638. Conjugated polymers via cyclopentannulation strategies. **K.N. Plunkett**, S. Bheemireddy, M.p. Hautzinger, X. Zhu, S. Somisetti, K. DuBay

10:00 POLY 639. Anionic polymerization of aziridines. **P.C. Mbarushimana**, P.A. Rupar

10:20 POLY 640. Withdrawn

10:40 POLY 641. *Ab initio* thermal conductivity evaluation of polymer systems. **K. Uchimura**, T. Ichibha, R. Maezono, K. Hongo

11:00 POLY 642. Facile synthesis of fluorine-substituted, alternating polylactides and their amphiphilic block copolymers. **C. Lee**, R. Khalifehzadeh, B.D. Ratner, A.J. Boydston

11:20 POLY 643. Cyclopolymerization of 1,2-dicarbodiimides. **C.U. Jayarathna**, E.H. De Silva, B.M. Novak

11:40 POLY 644. Synthesis and characterization of polyelectrolytes containing tetraarylphosphonium moieties by using diphenylphsophine as commercial building block. **W. Wan**, X. Yang, R. Smith

Section H
New Orleans Marriott Canal Street Audubon

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
J. Bohling, W. Gao, D.N. Haase, J. Tsavalas, W. Wu, *Organizers*
D.S. Germack, C. Lipscomb, *Organizers, Presiding*

8:00 POLY 645. Bulk and interfacial properties of acrylic emulsion-based pressure sensitive adhesives via microindentation probe tack. **M. Einsla**, W. Griffith, Q. Wang, M.L. Pacholski, S. Zhang, K.R. Shull

8:30 POLY 646. Withdrawn

9:00 POLY 647. Polymer colloids with improved re-dispersibility in alcohol based formulation. **F. Zeng**, W. Xu, K. Beshah, L. Bai, B. Yezer,, L. Chen, D. Schmidt, I. Shulman

9:20 POLY 648. Applications of polymer colloids in Waterborne coatings: Influences of composition and process designs on coatings performance properties: Tutorial. **W. Wu**

10:00 Intermission.

10:30 POLY 649. Colloidal particles for green printing technology. **Y. Song**

11:00 POLY 650. Development of photoactive inks for application in organic electronics. **E. Cloutet**

11:30 POLY 651. Property comparison between solvent-based and water-based epoxy-amine clear coatings. **M. Pramanik**, E. Kaya, D. Dellate, M. Blanton, J. Rawlins

Lignin: From Fundamentals to New Materials & Applications

Nanoscaled Materials from Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

WEDNESDAY AFTERNOON

Section A
New Orleans Marriott Canal Street Studio 6

International Symposium on Biorelated Polymers: Renewable Materials

Synthesis of Renewable Materials

Cosponsored by PMSE
A. Watts, *Organizer*
E.W. Cochran, E.C. Hagberg, R.T. Mathers, *Organizers, Presiding*

1:00 POLY 652. Synthesis of renewable polyurethanes derived from isohexides and furans: Stereochemical effects on mechanical and viscoelastic properties. **R.J. Kieber**, S. Silver, J.G. Kennemur

1:20 POLY 653. Withdrawn

1:40 POLY 654. Synthesis of high performance phthalonitrile resins from renewable resources. **M. Derradji**, A. Wang, W. Liu

2:00 POLY 655. Novel biomolecular design of N-boronated polybenzimidazole with single ion conductivity. **A. Nag**, M. Asif, R. Vedarajan, N. Matsumi, T. Kaneko

2:20 POLY 656. Emulsion-templated renewable resource polymers: Open-cell scaffolds and closed-cell encapsulation. L. Avraham, L. Wienstock, I. Berezovska, R. Sanguramath, **M.S. Silverstein**

3:00 Intermission.

3:30 POLY 657. Renewable materials constructed through mimicking biomineralization. **M.R. Hartings**

4:00 POLY 658. Bio-based thiol-ene polymers for use in battery applications: Synthesis and properties. **E.A. Baroncini**, J.F. Stanzione

4:20 POLY 659. Nature-derived renewable polymers to replace commodity plastics. **O. Nsengiyumva**, E. Sahmetlioglu, H. Nguyen, E. Gokturk, S.A. Miller

Section B
New Orleans Marriott Canal Street Studio 1

Polymer Optoelectronics

J.D. Azoulay, X. Gu, *Organizers*
Y.C. Simon, *Organizer, Presiding*

1:00 POLY 660. Development of electro-active inks for organic electronics. **E. Cloutet**

1:20 POLY 661. Strategies for triplet fusion upconversion. **A. Pun**, D.N. Congreve, L.M. Campos

1:40 POLY 662. Towards supramolecular systems for efficient triplet-triplet annihilation photon upconversion. **K. Moth-Poulsen**

2:10 POLY 663. Polypeptide-induced organization of semiconducting polymers into hybrid electroactive materials with enhanced photo-physical properties. **C. Rosu**, P. Russo, E. Reichmanis

2:30 POLY 664. Designing organic mixed conductors for bioelectronic applications. **J. Rivnay**

3:00 Intermission.

3:30 POLY 665. Design considerations for organic thermoelectric materials. **B.C. Schroeder**

4:00 POLY 666. Designing charge-neutral, non-conjugated radical polymers with high electrical conductivity values. **B.W. Boudouris**, V. Agarkar, Y. Joo

4:30 POLY 667. Multifunctional electronic materials for thin film devices. **S. Yoo**, E. Gomez

4:45 POLY 668. Multifunctional charge transfer-based supramolecular materials with tunable thermochromism. **T. Yuan**, M. Olson, L. Fang

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Biobased Materials

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
M. Gaborieau, *Presiding*

1:00 POLY 669. Diffusion and relaxometry NMR to study interactions between carbohydrates in ionic liquids. **M.E. Ries**, T. Budtova, W. Ezzawam

1:25 POLY 670. Starch/sucrose amorphous blends studied by low- and high-resolution solid state NMR. **M. Geppi**, F. Martini, G. Mencarini, G. Badolato-Bönisch, D.J. Hughes, J. Ubbink

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1:50 POLY 671. Insights into the heterogeneity of polysaccharides with solid-state NMR spectroscopy. J.J. Thevarajah, M.P. van Leeuwen, M. Heuls, A. Rouilly, R.M. Ward, E.P. Gilbert, R. Graf, P. Castignolles, **M. Gaborieau**

2:15 POLY 672. NMR analysis of compositionally heterogeneous polysaccharides. **H. Cheng**

2:40 Intermission.

2:55 POLY 673. Solid State NMR at high and low field for the characterization of bioplastics obtained from vegetable wastes. **R. Simonutti**, M. Mauri, G. Perotto

3:20 POLY 674. Analysis of C-H and N-H distances of amino acids and polypeptides by CP-VC method. **H. Kimura**, Y. Tsutsumi, J. Amoureux, A. Shoji

3:45 POLY 675. Characterization of microbial poly(β-glutamic acid) and its polymer complex by solid NMR. **S. Maeda**

4:10 POLY 676. Investigation of polypeptide structure-property relationship by proton (H1)/spin-lattice relaxation time (T1) nuclear magnetic resonance and pulsed gradient spin echo (PGSE). **C. Rosu**, E. Von Meerwall, D. Treleaven, P. Russo

Section D
New Orleans Marriott Canal Street
Studio 2

Paul J. Flory Polymer Education Award: Symposium in honor of Timothy P. Lodge

M.D. Ediger, *Organizer, Presiding*

1:00 POLY 677. Self-assembly of responsive polypeptide block copolymers. **D.A. Savin**

1:30 POLY 678. Complex lyotropic liquid crystalline sphere packings in aqueous dispersions of a diblock polymer. **M.K. Mahanthappa**

2:00 POLY 679. Using physical vapor deposition to produce structured glasses. **M.D. Ediger**

2:30 POLY 680. Hydrogen bonded complex in photo-initiated cationic polymerization of epoxides and oxetanes. **C.Y. Ryu**, S. Park

3:00 Intermission.

3:30 POLY 681. Functional polymeric ionic liquids. **R.A. Segalman**

4:00 POLY 682. Composition-dependent dynamics in polyelectrolyte complex coacervates. **J. Laaser**, F. Morin, J. Huang

4:30 POLY 683. Thermoreversible gelation of methylcellulose: Confounding what we teach in Polymers 101. **T.P. Lodge**, S. Morozova, P. Schmidt, F. Bates

Section E
New Orleans Marriott Canal Street
Studio 10

Adaptive Nanogels
Cosponsored by COLL
A. Fernandez-Nieves, T. Hoare, L.A. Lyon, D. Suzuki, *Organizers*
W. Richtering, *Organizer, Presiding*
D. Woell, *Presiding*

1:00 POLY 684. Adhesive microgels. **R.H. Pelton**

1:30 POLY 685. Soft microgels at liquid interfaces: model surfaces and emulsions. **V. Ravaine**

2:00 POLY 686. Functional hydrogel microspheres at the air/water interface. **D. Suzuki**, M. Takizawa, H. Minato, Y. Sazuka

2:30 POLY 687. Interface-mediated self-assembly of multifunctional core-shell microgels. K. Volk, T. Honold, **M. Karg**

3:00 Intermission.

3:30 POLY 688. Smart nanomembranes by electron beam cross-linking of copolymer microgels. **T. Hellweg**

4:00 POLY 689. Macroscopic aqueous foams stabilized by PNIPAM microgels. **M. Kühnhammer**, R. von Klitzing

4:20 POLY 690. Mechanical characterization of single microgels using atomic force microscopy nanoindentation. **J. Nicosia**, D. Chambers, A. Fernandez-Nieves, W. Lam, T. Barker

4:40 POLY 691. Monte Carlo simulations of weak polyampholyte microgels: pH-dependent ionization and volume change. C. Hofzumahaus, C. Strauch, **S. Schneider**

Section F
New Orleans Marriott Canal Street
Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*
J.A. Kalow, J.A. Reeves, *Presiding*

1:00 POLY 692. Photocontrol of crosslink exchange kinetics in hydrogels and vitrimers. **J.A. Kalow**

1:30 POLY 693. Photo-switchable plasticity in (photo)polymerized network polymers. **C. Bowman**, B. Worrell, M.K. McBride, G. Berg, C. Wang, L. Cox

2:00 POLY 694. Photo-sensitive multi-responsive structurally dynamic polymers. **S.J. Rowan**

2:30 POLY 695. Strong underwater adhesion of low modulus polyester adhesives is achieved with photochemical control of cohesive bonds. A. Narayanan, S. Kaur, Q. Liu, A.N. Dhinojwala, **A. Joy**

3:00 Intermission.

3:30 POLY 696. Photochemical grafting of functional copolymers with high abrasion resistance. **J.J. Locklin**

4:00 POLY 697. Driving polymer and surface modification using visible light. **J. Blinco**, P. Lederhose, C. Barner-Kowollik

4:30 POLY 698. Preparation of micro-patterned surfaces by the use of light-sensitive alkoxyamines. **Y. Guillaneuf**

Section H
New Orleans Marriott Canal Street
Audubon

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Cosponsored by ANYL, COLL, COMP, I&EC and PMSE
Financially supported by Wyatt Technology; Anton Paar USA, Inc.; The Dow Chemical Company; Arkema; Solvay
W. Gao, D.S. Germack, D.N. Haase, C. Lipscomb, W. Wu, *Organizers*
J. Bohling, J. Tsavalas, *Organizers, Presiding*

1:00 POLY 699. Opacifying polymer imaging: a new strategy for thermal printing. **A. Hejl**, B. Einsla, C. Chung

1:30 POLY 700. Waterborne coating formulations with poly (vinyl acetate) and acrylic latex blends utilizing design of experiments and high-throughput methodology. **P.S. Majumdar**, M.H. Keefe, K. Alderfer, B. Rowe, K. Oleksiak, M. Toth, K. Henderson, J. Sweeney

2:00 POLY 701. Altering friction reducer viscosities by controlling polymer concentration, brine composition and mixing energy. **C. Aften**

2:30 POLY 702. Post-polymerization molecular weight advancement in an acrylic latex adhesive and its effects on adhesive properties. **K. Schultz**, C. Lipscomb

3:00 Intermission.

4:00 POLY 703. Optimization of polymer-graphene nanoplatelet chemiresistive sensors for detection and discrimination of chemical warfare agents. **M.S. Wiederoder**, M. Weiss, E.C. Nallon, R. Paffenroth, V.P. Schnee, C.J. Bright, S.K. Mcgraw, J.R. Uzarski

Lignin: From Fundamentals to New Materials & Applications

Carbon Fibers & Chemicals from Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

WEDNESDAY EVENING

Section A
New Orleans Marriott Canal Street
Acadia

POLY/PMSE Plenary & Awards Event
Cosponsored by PMSE‡
T.H. Epps, *Organizer*
D. Gerbi, *Presiding*

5:30 Networking Reception.

6:00 POLY 704. Plenary lecture: Skin-inspired polymer electronic materials and devices. **Z. Bao**

6:40 Awards Presentation.
7:00 Reception.

THURSDAY MORNING

Section A
New Orleans Marriott Canal Street
Studio 6

International Symposium on Biorelated Polymers: Renewable Materials

Renewable Polyesters
Cosponsored by PMSE
A. Watts, *Organizer*
E.W. Cochran, E.C. Hagberg, R.T. Mathers, *Organizers, Presiding*

8:00 POLY 705. Cellulose ester and biodegradable polyester blends having improved properties. **J.H. Wang**, B. Zhou

8:30 POLY 706. Bio-based carboxylic acids as components of sustainable coating systems. **I. Hevus**, D.C. Webster

8:50 POLY 707. Polymersation of limonene and β-pinene derived monomers for the syntheiss of novel renewable polyesters. **M. Thomsett**, S.M. Howdle, R.A. Stockman

9:10 POLY 708. Attaching multiple B vitamins to polyesters. **R.T. Mathers**

9:40 POLY 709. Preparation and characterization of bio-based polyesters and polycarbonates derived from xylochemicals. **S. Curia**, J. Mauck, A. Bassett, J.F. Stanzione

10:00 Intermission.

10:30 POLY 710. Glyoxylate-containing block copolymer materials. D. Hewitt, **R.B. Grubbs**

11:10 POLY 711. Poly(ethylene terephthalate) mimics based on naturally derived starting material. **G. Short**, H. Donow, H. Nguyen, S.A. Miller

11:30 POLY 712. Characteristic of biodegradable polyester PHBH and water-soluble poly(vinyl alcohol) blend nanofibers. **R.A. Rebia**, T. Tanaka

Section B
New Orleans Marriott Canal Street
Studio 1

Polymer Optoelectronics

J.D. Azoulay, Y.C. Simon, *Organizers*
X. Gu, *Organizer, Presiding*
J. Tropp, *Presiding*

8:00 POLY 713. Designing high ductility polymers for stretchable electronics. **C.K. Luscombe**

8:20 POLY 714. Understanding polymer physics of conjugated polymers for future deformable semiconductors. **R. Xie**, R.H. Colby, E. Gomez

8:50 POLY 715. Directly measuring the complete stress–strain response of ultrathin organic electronic films. **X. Gu**, S. Zhang

9:10 POLY 716. Relationships between chain properties of the active layer and performance of polymeric electronic devices. **E. Gomez**

9:40 POLY 717. Hydrogen bonding in semiconducting polymers: Effect on self-assembly and mechanical properties. T. Nguyen, M.U. Ocheje, B.P. Charron, **S. Rondeau-Gagne**

10:00 Intermission.

10:30 POLY 718. Melt-processable semiconducting polymer blends. **J. Mei**

11:00 POLY 719. Printing semiconductor polymers to order: Critical roles of interfaces and fluid flow. **Y. Diao**

11:30 POLY 720. Synthesis of water-soluble ionic elastomers for stretchable

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organic electronics. **L.V. Kayser**, M.D. Russell, A.N. Stein, D.J. Lipomi

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Biobased Materials

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
Y. Suzuki, *Presiding*

8:00 POLY 721. Structure and dynamics of protein hydrogels. **P.A. Mirau**, M. Gupta, P. Dennis

8:25 POLY 722. Solid-state NMR studies of graphene-based systems and nano-mole-scale protein solid-state NMR using ultra-fast MAS. **Y. Ishii**

8:50 POLY 723. Targeting repeating subunits in elastin with strategic enrichment and solid-state NMR spectroscopy. **K.K. Kumashiro**, K. Ohgo, J. Djajamuliadi, C. Dabalos

9:15 POLY 724. Understanding block-copolymer micelle dynamics and molecular partitioning for tunable cargo encapsulation and delivery. **X. Li**, B.E. Kidd, T.J. Cooksey, M.L. Robertson, L.A. Madsen

9:40 Intermission.

9:55 POLY 725. NMR of silk. T. Asakura, **A. Nishimura**

10:20 POLY 726. Conformation and dynamic properties of silk fibroin in a silk gland. **Y. Suzuki**

10:45 POLY 727. Using magnetic resonance techniques to probe the structure and dynamics in synthetic & natural spider silks. **J.L. Yarger**, X. Shi, C. Guo, A. Lazaric, B. Cherry

11:10 POLY 728. Using NMR to probe the structure, dynamics and assembly of spider silk fibers. D. Onofrei, D. Stengel, G. Valdez, A. Villalba, B. Addison, **G.P. Holland**

Section D
New Orleans Marriott Canal Street Studio 5

Polymer Networks: Soft Gels to Stiff Networks
Cosponsored by PHYS, PMSE and SOCED
E. Chan, R.B. Moore, *Organizers*
S. Kundu, *Organizer, Presiding*

8:00 POLY 729. Elastomer organogels: Generating motion through crystallization of the swelling solvent. **K.A. Cavicchi**

8:30 POLY 730. Effects of poly(ethylene glycol) grafting density on the thermoreversible formation of a fibrous methylcellulose network. **S. Morozova**, P. Schmidt, F.S. Bates, T.P. Lodge

9:00 POLY 731. Withdrawn

9:20 POLY 732. Metamorphosis within polymer networks: Stress relaxation, network shape control and second-stage functionalization reactions. **M. Podgorski**, J. Sinha, B. Worrell, C. Bowman

9:40 POLY 733. Polymer networks with reversible and/or exchangable cross-links: Complete property recovery associated with cross-link density leading to fully reprocessable, recyclable networks and an approach to suppress creep in vitrimers. **J.M. Torkelson**, K. Jin, L. Li, X. Chen

10:00 Intermission.

10:30 POLY 734. Dynamic stimuli-responsive liquid crystal elastomers as actuating adhesives. **D.K. Schneiderman**, F. Etheridge, A. Metlay, S.J. Rowan

10:50 POLY 735. Free volume and gas transport studied in model elastomeric thiol-ene networks: Effect of crosslink density. **R. Ramakrishnan**, V. Vasagar, M.K. Hassan, S.I. Nazarenko

11:10 POLY 736. The coupling of polymer dynamics and water transport in cross-linked polymer membranes. **C.L. Soles**

11:30 POLY 737. Stimuli-responsively porating gels: Melting below glass transition. H. Gupta, N. Kuriakose, K. Lewis, S. Shendre, S. Venkatraman, **J. Texter**

11:50 POLY 738. Mechanistic insights into topological network impact on glass transition temperature. **J. Tsavalas**, P. Zhang, R. Biro

Section E
New Orleans Marriott Canal Street Studio 10

Adaptive Nanogels
Cosponsored by COLL
A. Fernandez-Nieves, T. Hoare, W. Richtering, D. Suzuki, *Organizers*
L.A. Lyon, *Organizer, Presiding*
L. De Laporte, *Presiding*

8:00 POLY 739. Degradable homogeneous microgels via self-assembly of reactive poly(N-isopropylacrylamide) oligomers. E. Mueller, D. Sivakumaran, R. Alsop, A. Scotti, M. Bleuel, M. Rheinstadter, W. Richtering, **T. Hoare**

8:30 POLY 740. Pathway-controlled complexity of metastable DNA microgels based on sequence-defined multiblock copolymers. **A. Walther**, R. Merindol, S. Loescher

9:00 POLY 741. Responsive and thermo-lockable hydrogels and nanogels. **F.M. Winnik**, X. Zhang, H. Ren, Y. Shi

9:20 POLY 742. Stimuli-responsive supramolecular microgels. **A. Pich**

9:40 POLY 743. Biodegradable and stimuli-responsive autodispersing polyurethanes. H. Gupta, **J. Texter**

10:00 Intermission.

10:30 POLY 744. Withdrawn

11:00 POLY 745. A responsive nanogel probe for ratiometric fluorescent sensing of pH and strain in hydrogels. **B. Saunders**

11:20 POLY 746. Superresolution fluorescence microscopy for the *in situ* visualization of compartmentalized microgels / nanogels. **D. Woell**, A. Oppermann, A. Gelissen, S. Centeno Benigno, O. Nevskyi, A. Purohit, L. Hoppe Alvarez

11:40 POLY 747. Non-reciprocal shape shifting microgels engine. **M. Ahmed**, H. Zhang, M. Moller

Section F
New Orleans Marriott Canal Street Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, *Organizers*
D.L. Patton, *Organizer, Presiding*
C.M. Reese, *Presiding*

8:00 POLY 748. Photoactive BODIPY polymer-based systems: Polymersomes for PDT and 2D & 3D micrometric surface patterning. V. Ibrahimova, G. Raffy, C. Fustin, J. Vincent, S. Lecommandoux, **N.D. McClenaghan**

8:20 POLY 749. Design and fabrication of mechanically stable polymer vesicles from crosslinkable linear amphiphilic triblock copolymers. **T. Chidanguro**, F. O'Dowd, Y.C. Simon

8:40 POLY 750. Polymer nanocomposites: In-situ photoconversion to nanoparticles with ketyl radicals. **R.C. Advincula**

9:10 POLY 751. Light-responsive polymersomes for spatially and temporally controlled release. **L. Beaute**, N.D. McClenaghan, S. Lecommandoux

9:30 POLY 752. Making and breaking polymers with light: Blue-light-mediated photoiniferter polymerization and polyketone degradation. **J.B. Matson**, K. Arrington

10:00 Intermission.

10:30 POLY 753. Photochemical release of doxorubicin linked through a thioacetal photocage in folate-targeted polymeric nanostructures. P.T. Wong, S. Tang, J. Cannon, **S. Choi**

10:50 POLY 754. Photochemical combinatorial discovery of antimicrobial polymers. S. Richards, E. Fullam, **M.I. Gibson**

11:20 POLY 755. Regioselective, C–H xanthylation as a platform technology for polyolefin functionalization. **F.A. Leibfarth**, E.J. Alexanian, J. Williamson, W. Czaplyski

Lignin: From Fundamentals to New Materials & Applications

Polymers & Resins from Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

Cyclic & Topologically Complex Polymers
Sponsored by PMSE, Cosponsored by POLY

THURSDAY AFTERNOON

Section A
New Orleans Marriott Canal Street Studio 6

International Symposium on Biorelated Polymers: Renewable Materials

Properties & Applications of Renewable Materials

Cosponsored by PMSE
A. Watts, *Organizer*
E.W. Cochran, E.C. Hagberg, R.T. Mathers, *Organizers, Presiding*

1:00 POLY 756. Cellulose nanocomposites. **J.P. Youngblood**, Y. Yoo, S. Peng, C. Clarkson

1:30 POLY 757. Effects of cellulose acetate butyrate on the crystallization of polylactic acid. **J. Kuang**, J.H. Wang, Y. Bai

1:50 POLY 758. Splitting of meniscus at air-LC interface of megamolecular polysaccharide and its theoretical evaluation. **G. Joshi**, K. Okeyoshi, M. Okajima, T. Kaneko

2:30 POLY 759. Stimuli responsive materials for personalized implants. **J. Foster**, J. Fallon, M. Bortner

3:00 Intermission.

3:30 POLY 760. Structure-property relationships of bio-based polyamides with super-high mechanical toughness. **Y. Yoshinaka**, S. Tateyama, K. Takada, Y. Funahashi, T. Kaneko

3:50 POLY 761. Bioproduct derived protective layers: Self-exfoliating reactive layers. **K.R. Carter**, Y. Li

4:30 POLY 762. Glycerol-based pressure sensitive adhesives: Synthesis and application. **F. Lin**, B. Claypool, N. Hernandez, A. Buss, E.W. Cochran

Section B
New Orleans Marriott Canal Street Studio 1

Polymer Optoelectronics

J.D. Azoulay, X. Gu, Y.C. Simon, *Organizers*
A.E. London, D. Weller, *Presiding*

1:00 POLY 763. Polyrhodamine: Towards the design of a new optical chemical sensory material. **C.N. Scott**, R.W. Wahalathantrige Don

1:15 POLY 764. Conjugated polymers containing boron and phosphorus. **P. Rupar**

1:45 POLY 765. Synthesis and optoelectronics of coplanar ladder polymers. **L. Fang**, M. Al-Hashimi

2:15 POLY 766. Synthesis of stable difuran derivatives with p-block elements bridge. **H. Cao**, P. Rupar

2:30 POLY 767. Functionalized graphene nanoribbons as semiconducting materials for organic electronics. **J. Morin**

3:00 Intermission.

3:30 POLY 768. Polarized soft X-ray scattering reveals chain orientation and domain size of conjugated block copolymer lamellae. **J. Litofsky**, M. Aplan, Y. Lee, E. Gomez

3:45 POLY 769. Optoelectronic properties of sequentially-processed, chemically-doped, controlled crystallinity conjugated polymer fllms. T. Scholes, T.

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Aubry-Komin, **B.J. Schwartz**

4:15 POLY 770. Polarizabilities of π-conjugated polymers revisited: Improved results from broken-symmetry, range-separated DFT. **B.M. Wong**, N.V. Ilawe, M.B. Oviedo

4:30 POLY 771. Using conjugated block copolymers to examine the dependence of charge transfer on conjugation length. **M.P. Aplan**, E. Gomez

4:45 POLY 772. Minimizing beam damage with antioxidants to enable high resolution imaging of conjugated polymers in the electron microscope. **B. Kuei**, E. Gomez

Section C
New Orleans Marriott Canal Street Studio 4

Structure & Dynamics of Materials via NMR Spectroscopy

Solution NMR of Polymers

Financially supported by ExxonMobil; Bruker; JEOL; 3M; MR Resources; NMR Service; Rototec-Spintech; Cambridge Isotope; New Era Enterprises
H. Cheng, A.D. English, *Organizers*
A. Whittaker, *Presiding*

1:00 POLY 773. Polymers from earth and space. **A. Rawal**

1:25 POLY 774. Solution properties of thermally sensitive macromolecules studied by high resolution NMR and MD simulations. C. Zhang, W. Li, L. Liu, J. Reid, S. Bernardi, D.J. Searles, H. Peng, A. Zhang, **A. Whittaker**

1:50 POLY 775. Characterization of photo-initiated living radical polymerization kinetics with *in-situ* NMR spectroscopy. **J. Battiste**, B. Gaddam, A. Lohse

2:15 POLY 776. NMR analysis of the stereoregularity of poly(lactic acid) through the use of selective solvents. **K. Suganuma**, M. Oshimura, T. Hirano, K. Ute, H. Cheng, T. Asakura

2:40 Intermission.

2:55 POLY 777. Multidimensional NMR studies of perfluoropolyether. H. Yin, F. Wu, J. Gu, P.L. Rinaldi, **X. Li**

3:20 POLY 778. Advanced NMR methods for determining sequence distributions in fluoropolymer elastomers. **H. Mason**, J. Vaughn, C. Plavchak, J.P. Lewicki, S.C. Chinn

3:40 POLY 779. Making NMR more accessible. **W. Hu**

4:05 POLY 780. Evaluating co-monomer sequence distribution in brominated syndiotactic polystyrene (sPS-Br) copolymers using ^{13}C NMR spectroscopy. **K.M. Felice**, R.B. Moore

4:25 POLY 781. Structure analysis of blockiness controlled poly (vinyl alcohol-co-vinyl acetate) by NMR. **Y. Kusaka**, M. Senoo, T. Hirano, K. Ute

Section D
New Orleans Marriott Canal Street Studio 5

Polymer Networks: Soft Gels to Stiff Networks

Cosponsored by PHYS, PMSE and SOCED
E. Chan, S. Kundu, *Organizers*
R.B. Moore, *Organizer, Presiding*

1:00 POLY 782. Enhanced elasticity and property modification of poly(acrylic acid) and other polyelectrolytes: Studying and modeling the effects of salts and ionic liquids added during synthesis on material behavior. **A.Y. Walker**, M.A. Vratsanos, N. Bedford, S.K. Kozawa, G.E. Wnek

1:20 POLY 783. Chain conformation in polyelectrolyte complexes, from solids to gels. **H.M. Fares**, Y. Ghoussoub, J. Delgado, V. Urban, J.B. Schlenoff

1:40 POLY 784. Gels and frameworks comprising of organic linkers and polyanionic clusters via non-covalent bonding towards membranes for filtration and separation. **L. Wu**

2:00 POLY 785. Soft-hard polymer gradient materials based on thermoreversible urea-siloxane networks. **E. Fuersattel**, R. Giesa, H. Schmidt

2:20 POLY 786. Metal-free borane hydrosilylation as a mild route to diverse silicones. **C. Sample**, S. Lee, S. Li, B. Versaw, C.J. Hawker

2:40 POLY 787. Molecular design strategies for recyclable, high-performance networked polymers based on new dynamic covalent bonding motifs. **B. Helms**, P. Christensen

3:00 Intermission.

3:30 POLY 788. Molecular ionic composites: Stiff solids with liquid-like ions inside. **L.A. Madsen**

4:00 POLY 789. Photocured networks from polyisobutylene macromers. **C. Parada**, R.F. Storey

4:20 POLY 790. Influence of processing conditions on morphological features in poly(ether ether ketone) gels and aerogels. **S. Talley**, R.B. Moore

4:40 POLY 791. Withdrawn

Section E

New Orleans Marriott Canal Street Studio 10

Adaptive Nanogels
Cosponsored by COLL
A. Fernandez-Nieves, T. Hoare, L.A. Lyon, W. Richtering, *Organizers*
D. Suzuki, *Organizer, Presiding*
A.J. Kuehne, *Presiding*

1:00 POLY 792. Ultra low crosslinked microgels are ordered in bulk and disordered in two-dimensions. **A. Scotti**, S. Bochenek, M. Brugnoni, M.A. Fernandez-Rodriguez, F. Schulte, J. Houston, A. Gelissen, L. Isa, W. Richtering

1:20 POLY 793. Cationic, anionic, or amphoteric dual pH/temperature-responsive degradable microgels via self-assembly of oligomeric precursor polymers for drug delivery. **E. Mueller**, A. Arezina, D. Sivakumaran, T. Hoare

1:40 POLY 794. Hydrophobically-modified poly(oligoethylene glycol methacrylate)-based nanogels for the delivery of anti-psychotic drugs to the brain. **M. Simpson**, Y. Katare, N. Smeets, R. Mishra, T. Hoare

2:00 POLY 795. Peptide-loaded microgels as antimicrobial surface coatings. **L. Nyström**, R. Nordstrom, A.A. Strömstedt, B. Saunders, R. Álvarez-Asencio, M.W. Rutland, M. Malmsten

2:20 POLY 796. Stratified hydrogels and architectural control of temperature response. **W.T. Higgins**, V.A. Kozlovskaya, A. Alford, J. Ankner, E.P. Kharlampieva

2:40 Intermission.

3:10 POLY 797. Poly(acrylic acid) microgels as carriers for antimicrobial peptides. **R. Nordstrom**, L. Nyström, O.C. Andrén, M. Malkoch, A. Umerska, M. Davoudi, A. Schmidtchen, M. Malmsten

3:30 POLY 798. Synthesis and functionalization of polymer nanoparticles. **K. Misichronis**, T. White, H.J. Martin, A.P. Sokolov, M.D. Dadmun, T. Saito

3:50 POLY 799. Hydrogel microspheres for selective separation of halogen compounds. **T. Kureha**, D. Suzuki

Section F
New Orleans Marriott Canal Street Studio 7

Photochemistry & Polymers

B.P. Fors, D. Konkolewicz, D.L. Patton, *Organizers*
D. Konkolewicz, A.M. Spokoyny, *Presiding*

1:00 POLY 800. Controlling photo-induced phase separation through kinetics and polymer architecture. **A. Guymon**, J.P. Scholte

1:30 POLY 801. Light intensity induced phase transitions in graphene oxide doped polyvinylidene fluoride. **O. Paul**, A. Joaquim, M. Eguakun, V. Petranovskii, Y. Barnakov, F. Williams

1:50 POLY 802. Light-controlled phase separation using different monomer compositions of a radical/cationic system. **E. Hasa**, J.L. Jessop, J.W. Stansbury, A. Guymon

2:10 POLY 803. Photoredox chemistry for efficient thiol-alkyne coupling and polymer synthesis. **D. Konkolewicz**, M. Allegrezza, A. Thompson, A. Kloster

2:30 POLY 804. Boron cluster photosensitizers and dopants. **A.M. Spokoyny**

3:00 Intermission.

3:30 POLY 805. PhotoRedox catalysts in polymerization reactions: Towards to high performances systems. **J. Lalevee**

4:00 POLY 806. Synthesis and kinetic studies of thiol – ene post-polymerization modification of poly(vinylmethylsiloxane). **S. Chatterjee**, B. You, A.S. Raymond, J.N. Albert

4:20 POLY 807. Thiol-trifluorovinyl ether (TFVE) photopolymerization: An on-demand synthetic route to semi-fluorinated polymer networks. B. Donovan, J. Ballenas, **D.L. Patton**

Section G
New Orleans Marriott Canal Street Beauregard

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*
G. Saenz, K.A. Stockmal, *Presiding*

1:00 POLY 808. Thermoplastic elastomers from one-component block copolymer grafted nanoparticles via surface-initiated RAFT polymerization. **Y. Huang**, Y. Zheng, A. Sarkar, Y. Xu, M. Stefik, B.C. Benicewicz

1:20 POLY 809. Synthesis of novel biorenewable poly(ether amide)s. **G. Saenz**

1:40 POLY 810. Durable coatings with low ice adhesion. **S.J. Moravek**

2:00 POLY 811. Blocky bromination of poly(ether ether ketone) in the gel-state as a platform for further functionalization. **L. Anderson**, R.B. Moore

2:20 POLY 812. Combination of anionic ring-opening and condensation reactions for the synthesis of aliphatic-aromatic copolyamides. **C. Bakkali-Hassani**, S. Carlotti

2:40 POLY 813. n-Heterocyclic carbene organocatalyzed ring-opening polymerization of n-tosyl aziridines using functional initiators and amino-alcohols as bifunctional and double headed initiators. **C. Bakkali-Hassani**, J. Vignolle, S. Carlotti, D. Taton, E. Rieger, F. Wurm

3:00 POLY 814. Withdrawn

Lignin: From Fundamentals to New Materials & Applications

Biochemical Modification of Lignin

Sponsored by CELL, Cosponsored by ENVR and POLY

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems
Sponsored by CELL, Cosponsored by ENVR and POLY

PMSE

Division of Polymeric Materials Science and Engineering

M. Becker, B. Olsen, C. Snyder, X. Jia and A. Norman, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Industrial Innovations in Polymer Science (see *I&EC*, Mon)

Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Aleksandr Zhukhovitskiy & Jeremiah A. Johnson (see *POLY*, Tue)

SOCIAL EVENTS:

Reception, 5:30 PM: Wed

BUSINESS MEETINGS:

Executive Meeting, 4:30 PM: Sun

Business Meeting, 5:00 PM: Mon

PMSE-POLY Coordination Meeting, 5:30 PM: Mon

‡*Cooperative Cosponsorship*

SUNDAY MORNING

Section A
New Orleans Marriott Canal Street
La Galerie 6

ACS Award in Applied Polymer Science: Symposium in honor Paula T. Hammond

Cosponsored by POLY and WCC
Financially supported by Eastman Chemical Company
L. Korley, N. Zacharia, *Organizers*
J.L. Lutkenhaus, *Organizer, Presiding*

8:00 PMSE 1. Layered biomimetic nanocomposites and property correlations. **N. Kotov**

8:30 PMSE 2. Permeability and selectivity of polyelectrolyte coacervate materials. **N. Zacharia**

9:00 PMSE 3. Amphiphilic multiblock polymers form controlled assemblies to promote oral drug delivery and cellular genome editing. **T.M. Reineke**

9:30 PMSE 4. Protein engineering of multi-functional biomaterials for regenerative medicine. **S.C. Heilshorn**

10:00 PMSE 5. Digital light synthesis to drive additive manufacturing: Convergence of hardware, software and molecular science. **J.M. DeSimone**

10:30 PMSE 6. Melt miscibility and solid-state properties of block copolymers of polyethylene with hydrogenated poly(x-norbornene)s. W. Mulhearn, **R.A. Register**

11:00 PMSE 7. Exploring biological barriers with nanoengineered particles. **F. Caruso**

11:30 PMSE 8. Effect of charge and charge distribution on protein-polymer coacervation. **B.D. Olsen**, S. Kim, H. Sureka, C.E. Mills

Section B
New Orleans Marriott Canal Street
La Galerie 4

Supramolecular Crosslink Dynamics & Polymer Materials Mechanics

N. Holten-Andersen, *Organizer*
E.A. Appel, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 PMSE 9. Dynamic bonding in nucleoporin-like protein materials. **B.D. Olsen**, D. Mai, Y. Yang

9:10 PMSE 10. Supramolecular polymers to supramolecular crosslinks: Progress in rational design of dynamic water soluble supramolecular architectures. **M.B. Baker**

9:30 PMSE 11. Biomimetic composite hydrogels with abiotic self-organizing nanofiber network. **L. Xu**, N. Kotov

9:50 PMSE 12. Hierarchical crosslinking and interpenetrated networks in the SLA/DLP 3D printing process. **R.C. Advincula**

10:10 Intermission.

10:25 PMSE 13. Mechanics of polymers with supramolecular cross-links. **C. Weder**

11:00 PMSE 14. pH-regulated viscoelastic properties of mussel-inspired telechelic hydrogel. **S. Cazzell**, N. Holten-Andersen

11:20 PMSE 15. Role of interfacial interactions in the toughening of supramolecular interpenetrating network elastomers. **C. Thompson**, S. Monemian, J. Covello, L. Korley

11:40 PMSE 16. Robust heterogeneous hydrogels based on supermolecular self-assembly with nanocellulose as dynamic crosslinkers. **K. Zhang**

Section C
New Orleans Marriott Canal Street
Studio 3

Polymers with Complex Architecture: From Synthesis to Self-Assembly

Financially supported by NSF, BASF, ExxonMobil, LG MMA, and Wyatt Technology, Department of Chemistry & Biochemistry at Florida State University
C.Y. Ryu, M. Seo, G. Stein, *Organizers*
J.G. Kennemur, *Organizer, Presiding*

8:30 PMSE 17. Bottlebrush copolymers: Morphological control through molecular architecture. **J. Rzayev**

9:00 PMSE 18. Brush-like elastomers: Super-soft and strain-stiffening. **S. Sheiko**

10:00 Intermission.

10:15 PMSE 19. Bottlebrush polymers as surface active additives in thin polymer films. **H. Mah**, T. Laws, H. Mei, R. Verduzco, G. Stein

10:35 PMSE 20. Synthesis of multifunctional bottlebrush polymers. R. Slegeris, B.A. Ondrusek, **H. Chung**

10:55 PMSE 21. Janus bottlebrush copolymers: A universal strategy enabling access to ultra-small phase separation. **Z. Guo**, A.N. Le, M. Zhong

11:15 PMSE 22. Synthesis of polyimide bottlebrush copolymers. **B. Swanson**, J. Rzayev

11:35 PMSE 23. Supramolecular assembly of nucleobase-containing bottlebrush polymers. **J. Foster**, Z. Hua, R.K. O'Reilly

Section D
New Orleans Marriott Canal Street
La Galerie 5

Synergy between Computation & Experiment in Accelerated Materials Discovery

S. Takeda, *Organizer*
V.A. Piunova, *Organizer, Presiding*

8:30 PMSE 24. Materials informatics & AI: Examples from polymer materials. **J.W. Pitera**

8:55 PMSE 25. Mission Innovation Challenge 6: A route for accelerated scientific discovery for energy materials. **A. Aspuru-Guzik**

9:20 PMSE 26. Accelerating polymeric database creation. **D. Audus**, R. Tchoua, K. Chard, L. Ward, J. Qin, J. Lequieu, J.J. De Pablo, I. Foster

9:45 PMSE 27. Scoping the polymer genome: The example of rational computation-guided polymer dielectrics design. **R. Ramprasad**

10:10 Intermission.

10:25 PMSE 28. Inverse design of novel polymeric materials through Bayesian machine learning and experimental design algorithms. **R. Yoshida**, G. Lambard, S. Wu, H. Yamada

10:50 PMSE 29. Computational material discovery: Machine learning approach to discover new chemical structures. **S. Takeda**, K. Masuda, H. Hsu, J.B. Heroux, T. Hama, V.A. Piunova, J.W. Pitera, D. Nakano

11:15 PMSE 30. Multiscale design of polymer nanocomposite dielectric materials: Electron traps in interphase regions. **C.M. Breneman**, T. Ratcliff, L. Schadler, R. Sundararaman, C. Brinson, A. Lin

11:40 PMSE 31. Integrated experimental and computational high-throughput screening for polymer photocatalysts. C. Meier, L. Turkani, R.S. Sprick, E. Berardo, K. Jelfs, **M.A. Zwijnenburg**, A.I. Cooper

Section E
New Orleans Marriott Canal Street
Studio 2

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Membranes for Water & Ion Transport

Cosponsored by DAC‡
Financially supported by North American Membrane Society
D. Bhattacharyya, C.M. Stafford, *Organizers*
I.C. Escobar, B.D. Freeman, *Organizers, Presiding*
S.A. Hesse, *Presiding*

8:00 PMSE 32. Performance effects of oxidant and halide concentration on aromatic network polyamide membranes. **J.A. Howarter**, M. Toomey

8:30 PMSE 33. Functional group quantification in polyamide membranes. T.J. Zimudzi, D.F. Sunday, S.V. Orski, E. Chan, M.A. Hickner, **C.M. Stafford**

9:00 PMSE 34. Formation of a crack-free, hybrid skin layer with tunable surface topography on elastomers using gel-liquid infiltration polymerization. **M. Wang**, J.M. Gorham, J. Killgore, M. Omidvar, H. Lin, F. DelRio, L. Cox, Z. Zhang, Y. Ding

9:30 PMSE 35. Variability in surface morphology of polyamide selective layers on thin-film composite membranes. **L.H. Arias Chavez**, S.B. Hornsby, P. Ranjan

10:00 Intermission.

10:30 PMSE 36. Ion specific effects in charged polymers for membrane applications. **G.M. Geise**

11:00 PMSE 37. Functionalized membranes for environmental and chemical synthesis applications. **D. Bhattacharyya**, S. Hernandez, H. Wan, S. Islam, A. Colburn, A. Aher

11:30 PMSE 38. Using electrochemical impedance spectroscopy to probe permselectivity in model polyamide membranes. D. Shaffer, K.E. Feldman, G.R. Stafford, E. Chan, **C.M. Stafford**

Section F
New Orleans Marriott Canal Street
Studio 8

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
D.H. Adamson, C. Powell, *Presiding*

8:30 PMSE 39. High refractive index and thermal stability UV-curable novel inorganic-organic acrylate nanocomposites. **K. Liu**, K. Hsieh

8:55 PMSE 40. Polymeric systems for the release of COS and H_2S. **C. Powell**, J. Foster, B. Okyere, M. Theus, J.B. Matson

9:20 PMSE 41. Effect of process pathway on microstructure development in epoxy thermoset resins. **J. Bates**, D. Nepal, H. Koerner, J.S. Wiggins, G. Kedziora, C. Reynolds, S. Tucker, E. Barjasteh

9:45 PMSE 42. Effect degree of oxidation has on graphene oxide polymer nanocomposite properties. **H.V. Kumar**, C.D. Liyanage, V. Vasu, D.H. Adamson

10:10 Intermission.

10:25 PMSE 43. Graphene oxide nanoplatelets embedded polyamide thin films for water desalination. **M. Abbaszadeh**, S. Kundu

10:50 PMSE 44. Self-assembled hexagonal boron nitride as a 3D polymerization scaffold. S.P. Ward, C.M. Chapman, Z. Cui, **D.H. Adamson**

11:15 PMSE 45. Synthesis of polymer particle sunscreens. **D.A. Loy**, N.P. Nanayakkara

11:40 PMSE 46. Controlled polymer synthesis and grafting architectures in continuous flow polymerizations. **R.C. Advincula**

Section G
New Orleans Marriott Canal Street
Studio 9

Clay-Polymer Composites: Nanoclays & Other Natural Nanoparticles

Polymer-Clay Nanocomposites

Financially supported by Applied Minerals, Inc.; Zibo Zhangdian Oriental Chemical Co., Ltd.
N. Kotov, E. Ruiz-Hitzky, A. Takahara, L. Zhang, *Organizers*
Y.M. Lvov, *Organizer, Presiding*

8:00 PMSE 47. Clay-enabled, environmentally-benign flame retardant nanocoatings. **J.C. Grunlan**, R.J. Smith, K. Holder

8:30 PMSE 48. Nanoarchitectonics for functional materials: Nanosheet-capsule, hole-in-cube, cube with antenna, and so on. **K. Ariga**, L. Shrestha

9:00 PMSE 49. Simulation and experimental studies of clay/elastomer nanocomposites. **L. Zhang**, X. Wu, R.

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Wang, J. Liu, Y. Fu, X. Zhou

9:30 PMSE 50. Biodegradable polymer/clay nanocomposites. **C.S. Ha**

10:00 Intermission.

10:10 PMSE 51. Molecularly engineered, light-adaptive self-assembled nacre-mimetics. **A. Walther**

10:40 PMSE 52. High gas barrier and stretchability in hydrogen-bonded multilayer nanobrick wall thin films. **S. Qin**, Y. Song, M. Floto, J.C. Grunlan

11:10 PMSE 53. Drug-clay nanohybrid systems for advanced drug delivery: Emerging research area in nanomedicine. **J. Choy**

International Symposium on Biorelated Polymers: Tutorial
Sponsored by POLY, Cosponsored by PMSE

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
Sponsored by POLY, Cosponsored by PHYS and PMSE

Polymer Applications & Characterization in Medical Device & Pharmaceutical Industries
Sponsored by POLY, Cosponsored by PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

SUNDAY AFTERNOON

Section A
New Orleans Marriott Canal Street
La Galerie 6

ACS Award in Applied Polymer Science: Symposium in honor Paula T. Hammond

Cosponsored by POLY and WCC
Financially supported by Eastman Chemical Company
L. Korley, J.L. Lutkenhaus, *Organizers*
N. Zacharia, *Organizer, Presiding*

1:30 PMSE 54. Order, disorder and mechanical properties of graft-block copolymers. **F.S. Bates**

2:00 PMSE 55. How water, salt, and pH universally influence the glass transition in polyelectrolyte complexes. Y. Zhang, P. Batys, M. Sammalkorpi, **J.L. Lutkenhaus**

2:30 PMSE 56. Top-down chemistry: Functional materials by modification of carbon nanomaterials. **T.M. Swager**

3:00 Intermission.

3:15 PMSE 57. Micellar temperature-responsive layer-by-layer assemblies. **S.A. Sukhishvili**, A. Kumarimaduvu Palanisamy, V. Albright

3:45 PMSE 58. Hierarchy-mediated mechanics in peptide-polyurea hybrids. **L. Korley**, L.E. Matolyak

4:15 PMSE 59. Designing soft electronics and their applications in biointerfaces. **Z. Bao**

4:45 PMSE 60. Nanolayered multicomponent particles for targeted tissue transport and combination therapies. **P.T. Hammond**

Section B
New Orleans Marriott Canal Street
La Galerie 4

Supramolecular Crosslink Dynamics & Polymer Materials Mechanics

E.A. Appel, *Organizer*
N. Holten-Andersen, *Organizer, Presiding*

1:30 PMSE 61. Dynamic crosslinked polymer networks for electronic materials and devices. **Z. Bao**

2:05 PMSE 62. Reprocessable, reprogrammable shape-memory polymer networks via dynamic thia-Michael addition. **K.M. Greenman**, S.J. Rowan

2:25 PMSE 63. Low-molecular-weight, high-mechanical-strength, and solution-processable telechelic polyetherimide end-capped with ureido-pyrimidinone. K. Cao, **G. Liu**

2:45 PMSE 64. Super-stretchable polymeric elastomers with healable property and recoverable functionality. **P. Cao**, B. Li, A.P. Sokolov, T. Saito

3:05 Intermission.

3:20 PMSE 65. Engineering dynamic behavior in protein networks. **L.J. Dooling**, D.A. Tirrell

3:55 PMSE 66. Investigation of supramolecular association dynamics on the deformation mechanics of polymer-grafted nanocomposites. **A. Tibbits**, K. Park, J. Streit, L.F. Drummy, R. Vaia

4:15 PMSE 67. Reversibly tunable hydrogels by photocontrolling dynamic covalent chemistry. **J. Accardo**, J.A. Kalow

4:35 PMSE 68. Optomechanical coupling for the study of the dynamic mechanical properties of metal-coordinate gels. **I. Mahmad Rasid**, B.D. Olsen, N. Holten-Andersen

4:55 Concluding Remarks.

Section C
New Orleans Marriott Canal Street
Studio 3

Polymers with Complex Architecture: From Synthesis to Self-Assembly

Financially supported by NSF, BASF, ExxonMobil, LG MMA, and Wyatt Technology, Department of Chemistry & Biochemistry at Florida State University
J.G. Kennemur, C.Y. Ryu, M. Seo, *Organizers*
G. Stein, *Organizer, Presiding*

1:30 PMSE 69. Organization and dynamics of compositionally-tuned polymer grafted nanocomposites. **M. Kilbey**, D.P. Street, R.I. Ramirez, J. Sangoro, J.M. Messman

2:00 PMSE 70. PRISM theory and molecular simulations studies linking polymer architecture to structure and thermodynamics in polymer nanocomposites and polymer solutions. **A. Jayaraman**

2:30 PMSE 71. Molecular and nanostructure engineering of polymer semiconductors. **E. Egap**

3:00 Intermission.

3:15 PMSE 72. Nanoporous polymer syntheses from aqueous lyotropic liquid crystals. **M.K. Mahanthappa**

3:45 PMSE 73. Information-directed assembly of molecular ladders bearing boronate ester rungs. **M. Dunn**, T. Wei, T.F. Scott

4:05 PMSE 74. Sol-gel polymerization to produce hierarchically porous monoliths for fixed bed catalysis. T.V. Kotbagi, R. Adhikari, J. Hudspeth, **M.G. Bakker**

4:25 PMSE 75. Single-digit nanometer designer block copolymers to balance surface free energies in thin films for perpendicular orientation control. **Y. Yoshimura**, Y. Nabae, T. Hayakawa

4:45 PMSE 76. PeptoPlexes: Using tri- or tetrablock copolypept(o)ides for the synthesis of non-self-replicating synthetic viruses. **M. Barz**

Section D
New Orleans Marriott Canal Street
La Galerie 5

Synergy between Computation & Experiment in Accelerated Materials Discovery

V.A. Piunova**,** *Organizer*
S. Takeda, *Organizer, Presiding*

1:30 PMSE 77. The materials genome initiative: What's happened? What's next? **E.K. Lin**

1:55 PMSE 78. Data mining for electromechanical and phase change properties of over 1000 2D materials. **E.J. Reed**

2:20 PMSE 79. Monte Carlo tree search for designing novel molecules and materials. **K. Tsuda**

2:45 PMSE 80. Accelerated experimental materials discovery through integration with theory and artificial intelligence. **J. Gregoire**

3:10 Intermission.

3:25 PMSE 81. Accelerated discovery of polymers for nucleic acid delivery using combinatorial synthesis and chemical informatics. **K. Rege**

3:50 PMSE 82. Experiment-inspired modeling to help understand and guide the design of formulations for polymer assisted drug delivery. **W.C. Swope**, A. Carr, J.E. Rice, V.A. Piunova

4:15 PMSE 83. Correlating solvated structure and GPC data for conjugated polymers. **A. Kleinschmidt**, S. Root, L.V. Kayser, C. Dhong, D.J. Lipomi

4:40 PMSE 84. Using computation to guide the development of novel polymeric ligands: Pyridine-terminated poly(3-hexyl thiophene)s to stabilize P3HT/nanocrystal blends. **M. Kilbey**, W.M. Kochemba, B. Sumpter

5:05 PMSE 85. Poly(3-hexylthiophene) synthesis: Understanding nickel-mediated transmetalation with Grignard reagents. **A. Vitek**, A. Leone, P.M. Zimmerman, A.J. McNeil

Section E
New Orleans Marriott Canal Street
Studio 2

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Novel Membranes & Membrane Functionalization

Cosponsored by DAC‡
Financially supported by North American Membrane Society
I.C. Escobar, B.D. Freeman, *Organizers*
D. Bhattacharyya, C.M. Stafford, *Organizers, Presiding*

1:15 Introductory Remarks.

1:20 PMSE 86. Toward structure-by-design polymer-brush modified membranes. J.J. Keating, **G. Belfort**

2:00 PMSE 87. Selective modification of membrane pore and external surfaces. A. Sengupta, A. Vu, X. Qian, **S. Wickramasinghe**

2:30 PMSE 88. Preparation of brush-modified membranes via a grafting through brush growth approach. **N.H. Vy**, D.H. Adamson

3:00 Intermission.

3:30 PMSE 89. Block copolymer-directed self-assembly and non-solvent-induced phase separation (SNIPS) derived porous functional materials for advanced separations. **S.A. Hesse**, J. Werner, P.A. Beaucage, K. Barteau, K.E. Fritz, U.B. Wiesner

4:00 PMSE 90. Structure, properties and performance of sulfonated pentablock terpolymer membranes as a function of hydration cycles. **D.V. Truong**, G. Stein, H. Ardebili, M. Kammoun

4:30 PMSE 91. Nanoporous membranes via *in-situ* self-assembly for scalable manufacture. **D. Weller**, L. Galuska, X. Gu

Section F
New Orleans Marriott Canal Street
Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

‡*Cooperative Cosponsorship*

1:30 Introductory Remarks.

1:40 PMSE 92. Advances in the synthesis and purification of cyclic polymers. **S.M. Grayson**, F.M. Haque, R. Elupula

2:10 PMSE 93. Towards quantitative macrocyclizations by original synthetic approach and characterization methods. **O.R. Coulembier**, T. Josse

2:40 PMSE 94. Multi-Gram scale synthesis of high molecular weight cyclic polyethylene glycol. C. Hoevelmann, R. Zorn, D. Richter, **J. Allgaier**

3:00 Intermission.

3:10 PMSE 95. Novel ring-closure methods for preparing cyclic polymers. **K. Zhang**

3:40 PMSE 96. Selective cyclic polymer synthesis via topology transformation. **T. Takata**

4:10 PMSE 97. Reprogramming the conformation of single chain nanoparticles. **C. Barner-Kowollik**

4:40 PMSE 98. Novel synthetic pathway for multicyclic poly(δ-caprolactone). Y. Mato, K. Honda, T. Isono, **T. Satoh**

5:10 PMSE 99. Synthesis of cyclic polymers prepared directly from dibrominated precursors. **E.S. Tillman**

Section G
New Orleans Marriott Canal Street
Studio 9

Clay-Polymer Composites: Nanoclays & Other Natural Nanoparticles

Polymer-Plate Nanoparticle Composites

Financially supported by Applied Minerals, Inc.; Zibo Zhangdian Oriental Chemical Co., Ltd.
N. Kotov, Y.M. Lvov, E. Ruiz-Hitzky, A. Takahara, *Organizers*
L. Zhang, *Organizer, Presiding*

1:30 PMSE 100. Multiscale biomimetic nanocomposites. **N. Kotov**

2:00 PMSE 101. Multifunctional nanoparticle-porous polymer foam composites: Applications in chemical decontamination and military medicine. **C.L. McGann**, B. Streifel, S.L. Giles, G.C. Daniels, J. Lundin, J.L. Miranda-Zayas, R. Balow, J.H. Wynne

2:30 PMSE 102. Withdrawn

3:00 PMSE 103. Graphene networks and their conductive nanocomposites. **Z. Yu**

3:30 PMSE 104. Rubber/graphene composites: Interface, hybridization and tire application. **B. Guo**, Z. Yang, S. Wu, Z. Tang, L. Zhang

4:00 PMSE 105. Polymer-clay nanocomposite coatings as efficient, environment-friendly surface pretreatments. **P.C. Suarez Martinez**, J. Robinson, H. An, R.C. Nahas, D. Cinoman, J.L. Lutkenhaus

4:30 PMSE 106. House of card nanostructuring in nanoclay-graphene in oil-water separators. **R.C. Advincula**

International Symposium on Biorelated Polymers: Tutorial
Sponsored by POLY, Cosponsored by PMSE

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
Sponsored by POLY, Cosponsored by PHYS and PMSE

Polymer Applications & Characterization in Medical Device & Pharmaceutical Industries
Sponsored by POLY, Cosponsored by PMSE

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

MONDAY MORNING

Section A
New Orleans Marriott Canal Street
La Galerie 6

ACS Award in Polymer Chemistry: Symposium in honor C. Grant Willson

Cosponsored by POLY
Financially supported by ExxonMobil Chemical Company; IBM
M.A. Hillmyer, *Organizer, Presiding*

8:50 Introductory Remarks.

9:00 PMSE 107. Advances in miktoarm star polymer design, synthesis, and self-assembly. **C. Bates**

9:25 PMSE 108. Separation of carbon dioxide and light hydrocarbons using norbornene-based polymeric membranes. **B.K. Long**, C. Maroon, K.R. Gmernicki, M. Higgins, T. Hong, T. Saito, N. Belov, Y.P. Yampolskii

9:50 PMSE 109. What good is monodispersity? Some applications of dendrimers towards mass spectrometry. **S.M. Grayson**

10:15 Intermission.

10:30 PMSE 110. Photochemically directing surface energy driven Marangoni convection to pattern polymer films. **C.J. Ellison**

10:55 PMSE 111. Mono(μ-oxo)-dialuminum (MOD) initiated polymerization of epoxides to new functional materials. **N.A. Lynd**

11:20 PMSE 112. VOLCAT: The development of a zero-waste catalytic recycling process for post-consumer PET. **R.D. Allen**

11:45 PMSE 113. Detecting and manipulating single DNA biopolymers with fluidic nanochips. **Q. Lin**

Section B
New Orleans Marriott Canal Street
La Galerie 4

Advances in Macromolecular Science & Engineering: Symposium in honor of David Schiraldi

Q. Lin, *Organizer*
L. Korley, J.K. Pokorski, *Organizers, Presiding*

8:15 PMSE 114. Designing high performance engineering polymers: From polyesters for packaging to polyureas for agriculture. R.J. Mondschein, J.M. Dennis, A.M. Pekkanen, L. Steinberg, M. Hegde, K.A. Valentine, C. Arrington, J. Wolfgang, S.R. Turner, **T.E. Long**

8:45 PMSE 115. Developments in textile, multifunctional, and carbon fibers. **S. Kumar**

9:15 PMSE 116. Cononsolvency of poly(N-isopropylacrylamide) (PNIPAM) and its analogs in water/alcohol mixtures. **M.J. Hore**, X. Lang

9:45 PMSE 117. Fundamental investigations into the cross linking of polyethylene. S.C. Sarngadharan, M. Conley, J. Faris, M. Malone, F.S. Mohammed, C. Winslow, H. Eldridge, J.M. Cogen, B.I. Chaudhary, P. Pollet, **C.L. Liotta**

10:15 Intermission.

10:30 PMSE 118. Oxygen and moisture barrier from polyelectrolyte-clay nanocoatings. **J.C. Grunlan**

11:00 PMSE 119. Unexploited approaches to improved polymer performance. **M. Jaffe**

11:30 PMSE 120. Copolyesters containing 4,4'-bibenzoate and 3,4′-bibenzoate units. **S.R. Turner**, H.E. Edling, H. Liu, R.J. Mondschein, T.E. Long, H. Sun, D.A. Schiraldi

Section C
New Orleans Marriott Canal Street
Studio 3

Polymers with Complex Architecture: From Synthesis to Self-Assembly

Financially supported by NSF, BASF, ExxonMobil, LG MMA, and Wyatt Technology, Department of Chemistry & Biochemistry at Florida State University
J.G. Kennemur, C.Y. Ryu, M. Seo, G. Stein, *Organizers*
M. Seo, *Organizer, Presiding*

8:00 PMSE 121. Self-assembly of end-functionalized block copolymers. **M. Park**

8:30 PMSE 122. Preferred domain orientation in block copolymer fibers after solvent annealing. **G. Liu**, Z. Zhou, K. Cao, X. Chen

9:00 PMSE 123. Switchable amphiphile self-assembly implementing molecular selectivity of PMMA triple helix formation. **A. Knight**, J. Ren, C.J. Hawker

9:20 PMSE 124. Versatile synthesis of miktoarm star block polymers. **M. Schulze**, R. Lewis, A. Anastasaki, C. Bates, C.J. Hawker

9:40 PMSE 125. Nanostructured dendrimers: Towards nanowires, nanoparticles, and virus assemblies. **R.C. Advincula**

10:10 Intermission.

10:25 PMSE 126. Synthesis and properties of nanotubes from cyclic peptide / polymer conjugates. **S. Perrier**

10:55 PMSE 127. Understanding the role of secondary structures in determining temperature sensitivity of peptide amphiphiles. **U. Sridhar**, P. Prasad, S. Thayumanavan

11:15 PMSE 128. Microstructure-property relationship of polymeric wormlike micelles in a protic ionic liquid. **R. Chen**, C. Lopez-Barron, N.J. Wagner

11:35 PMSE 129. Topology effect on protein-polymer block copolymers self-assembly. **T. Suguri**, B.D. Olsen

Section D
New Orleans Marriott Canal Street
La Galerie 5

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

I. Hamerton, H. Ishida, *Organizers*
P. Froimowicz, *Organizer, Presiding*
B. Lochab, *Presiding*

8:00 Introductory Remarks.

8:05 PMSE 130. Recent progress and future direction of polybenzoxazine reseach. **H. Ishida**

8:45 PMSE 131. Low-surface-energy property of polybenzoxazine. **S. Kuo**

9:20 PMSE 132. Phloretic acid as an alternative to the phenolation of aliphatic hydroxyls for the elaboration of polybenzoxazine. A. Trejo-Machin, L. Puchot, R. Quintana, **P. Verge**

9:50 PMSE 133. Novel hyperbranched benzoxazine: Synthesis and properties. **L. Wenbin**, A.Q. Dayo, J. Wang, W. Cai

10:10 Intermission.

10:25 PMSE 134. Polybenzoxazines – precursors of carbon matrices for electrocatalyst immobilization. **C. Andronescu**, S. Barwe, W. Schuhmann

10:55 PMSE 135. Synthesis and properties of new heterocyclic polybenzoxazine thermosets. **N. Ramdani**

11:15 PMSE 136. Polybenzoxazine-silica nanocomposites: Combined polymer-silica layer in the composite. J. Lee, T. Takeichi, **R. Saito**

11:35 PMSE 137. Oxidative ring-fusion

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aromatization and its role to pyrolytic carbonization of polybenzoxazines and other phenolic resins. **N. Leventis**, S. Donthula, H. Majedi Far, S. Mahadik-Khanolkar, C. Mandal, A.M. Saeed, C. Sotiriou-Leventis

Section E
New Orleans Marriott Canal Street Studio 2

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Membranes for Gas & Small-Molecule Separations

Cosponsored by DAC‡
Financially supported by North American Membrane Society
D. Bhattacharyya, I.C. Escobar, B.D. Freeman, C.M. Stafford, *Organizers*
L.H. Arias Chavez, G. Geise, *Presiding*

8:15 Introductory Remarks.

8:20 PMSE 138. Rubbery organic frameworks-tuning the gas-diffusion through dynameric membranes. **M. Barboiu**

9:00 PMSE 139. Strong adsorption of propylene helps propane/propylene separation through Ag^+-exchanged X-type zeolite membrane. M. Sakai, Y. Sasaki, **M. Matsukata**

9:30 PMSE 140. CO_2-philic polymer membranes for high flux CO_2 separation. T. Hong, P. Cao, B. Li, C. Smith, S.M. Mahurin, A.P. Sokolov, **T. Saito**

10:00 Intermission.

10:30 PMSE 141. Facile routes to enhance the selectivity of PDMS membrane-based gas separations. **D. Ahn**, **A. Greiner**, J.F. Thompson, A.N. Lichtor, J.S. Hrabal

11:00 PMSE 142. Withdrawn

11:30 PMSE 143. Polyimides with phosphaphenanthrene skeleton: Gas permeation study and molecular dynamics simulations. **S. Banerjee**, R. Chatterjee, S. Bisoi, V. Padmanabhan

Section F
New Orleans Marriott Canal Street Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

8:00 PMSE 144. Topological polymer chemistry designing macromolecular graph constructions. **Y. Tezuka**

8:30 PMSE 145. Cyclic polymers in polymer networks. J. Wang, B.D. Olsen, **J.A. Johnson**

9:00 PMSE 146. Topologically complex peptides from plants as tools for the development of eco-friendly drugs and agrichemicals. **D. Craik**

9:30 PMSE 147. Cyclization of peptides by multicomponent reactions. **D.G. Rivera**

10:00 Intermission.

10:10 PMSE 148. Solution and bulk properties of densely packed multicyclic polymers. **M. Monteiro**

10:40 PMSE 149. Precision constructions of topological and functional cyclic polymers. **Z. Zhang**, Z. Huang, N. Zhou, X. Zhu

11:10 PMSE 150. Progress in the synthesis and characterization of polyesters to demonstrate unique physical properties. **F.M. Haque**, G. Kelly, A. Bergeson, J. Albert, S.M. Grayson

11:30 PMSE 151. How closed loops impact melt surface fluctuations and surface segregation in blends. **M.D. Foster**

Section G
New Orleans Marriott Canal Street Studio 9

Clay-Polymer Composites: Nanoclays & Other Natural Nanoparticles

Clay Nanotubes & Nanofiber Composites

Financially supported by Applied Minerals, Inc.; Zibo Zhangdian Oriental Chemical Co., Ltd.
N. Kotov, Y.M. Lvov, E. Ruiz-Hitzky, L. Zhang, *Organizers*
A. Takahara, *Organizer, Presiding*

8:00 PMSE 152. Withdrawn

8:30 PMSE 153. Halloysite nanotubes as versatile material for conservation of cultural heritage. V. Bertolino, G. Cavallaro, **G. Lazzara**, S. Milioto, F. Parisi, R. Fakhrullin

9:00 PMSE 154. Halloysite/biopolymer composites for intracellular drug delivery and tissue engineering platforms. E. Naumenko, I. Guryanov, E. Rozhina, A. Novikov, **R. Fakhrullin**

9:30 PMSE 155. Self-assembly approach in halloysite nanotube composites. **Y.M. Lvov**, V. Vinokurov, R. Fakhrullin

10:00 Intermission.

10:10 PMSE 156. Withdrawn

10:40 PMSE 157. Synthesis of core-shell halloysite-chalcogenides based nanocomposites and its application in photocatalysis. **A. Stavitskaya**, D. Logvinenko, F. Pouresmaeil, Y.A. Darrat, V. Vinokurov

11:10 PMSE 158. Withdrawn

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers

Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

Integrating Polymer Science in the Curriculum
Sponsored by POLY, Cosponsored by CHED and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

MONDAY AFTERNOON

Section A
New Orleans Marriott Canal Street La Galerie 6

ACS Award in Polymer Chemistry: Symposium in honor C. Grant Willson

Cosponsored by POLY
Financially supported by ExxonMobil Chemical Company; IBM
M.A. Hillmyer, *Organizer, Presiding*

1:40 PMSE 159. Using bioinspired polypeptoids to make hierarchical, chiral structures and functional surfaces. **R.A. Segalman**, E. Davidson, A. Patterson, R.N. Zuckermann

2:05 PMSE 160. Realizing 5.4 nm full pitch lamellar microdomains by a solid-state transformation. **T.P. Russell**, D. Yu, J.K. Mapas, H. Kim, J. Choi, J. Rzayev

2:30 PMSE 161. 2D and 3D nanostructures by block copolymer self-assembly. **C.A. Ross**

2:55 Intermission.

3:10 PMSE 162. Metal-free controlled polymerizations. **C.J. Hawker**

3:35 PMSE 163. Synthesis of polymers utilizing ROMP processes. **R.H. Grubbs**

4:00 PMSE 164. Nanoporous thermosets by crosslinking block polymers in the disordered state. **M.A. Hillmyer**

4:25 Introduction of Awardee.
4:30 PMSE 165. Award Address (ACS Award in Polymer Chemistry Sponsored by the ExxonMobil Chemical Company). Polymer chemistry for microelectronics. **C.G. Willson**

Section B
New Orleans Marriott Canal Street La Galerie 4

Advances in Macromolecular Science & Engineering: Symposium in honor of David Schiraldi

L. Korley, J.K. Pokorski, *Organizers*
Q. Lin, *Organizer, Presiding*
R.C. Advincula, *Presiding*

1:30 PMSE 166. Accessing innovative porous polymers through emulsion templating. **M.S. Silverstein**

2:00 PMSE 167. Practical consideration of freeze-dried, low density polymeric composites. **M. Gawryla**

2:30 PMSE 168. Nanomaterials in 3D: A 20-year adventure from mechanically strong polymer-crosslinked aerogels to porous metals and ceramics. **N. Leventis**

3:00 Intermission.

3:15 PMSE 169. Ion transport in charged polymer membranes. **B.D. Freeman**

3:45 PMSE 170. New layered and porous polymeric systems and applications. **E. Baer**

4:15 PMSE 171. From polyester to aerogels, flammability and back. **D.A. Schiraldi**

Section C
New Orleans Marriott Canal Street Studio 3

Polymers with Complex Architecture: From Synthesis to Self-Assembly

Financially supported by NSF, BASF, ExxonMobil, LG MMA, and Wyatt Technology, Department of Chemistry & Biochemistry at Florida State University
J.G. Kennemur, C.Y. Ryu, M. Seo, G. Stein, *Organizers*
G. Liu, *Presiding*

1:30 PMSE 172. Synthesis of highly branched functional polymers by radical (co)polymerization of crosslinkers or inimers. **N.V. Tsarevsky**

2:00 PMSE 173. Nanostructured polymeric materials via polymerization-induced microphase separation towards separation and energy applications. **M. Seo**

2:30 PMSE 174. Synthesis and morphological investigations of complex multiblock copolymers architectures. **R. Gupta**, M. Misra, G. Vanderwoude, A. Shi, F. Escobedo, E. Coughlin

2:50 PMSE 175. Synthesis of multi-block polymer brushes creating nano strings of pearls structures. **Y. Wang**

3:10 Intermission.

3:25 PMSE 176. Polymers with complex porous architectures and complex macromolecular architectures through emulsion templating. S. Israel, T. Zhang, R. Mahroum, S. Feldman, **M.S. Silverstein**

3:55 PMSE 177. Thin film phase behavior and domain spacing of ternary homopolymer/block copolymer blends. **M. Uddin**, B. Lwoya, A. Goodson, A.S. Raymond, J. Albert

4:15 PMSE 178. Experimental and computational exploration of ABCA′ tetrablock terpolymer morphologies. **M.R. Radlauer**, A. Arora, M. Matta, K.D. Dorfman, F.S. Bates, M.A. Hillmyer

4:35 PMSE 179. Entropy induced diverse phase transitions of giant surfactant via rigid-rod junctions. **W. Shan**, S.Z. Cheng

4:55 PMSE 180. Mesoscale block copolymers. **D.M. Barber**, T. Emrick, A. Crosby

Section D
New Orleans Marriott Canal Street La Galerie 5

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

P. Froimowicz, I. Hamerton, *Organizers*
H. Ishida, *Organizer, Presiding*
S. Kuo, *Presiding*

1:30 PMSE 181. Sustainable

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benzoxazines: Efficient co-monomers for inverse vulcanization. **B. Lochab**, M. Monisha

2:00 PMSE 182. Chemical design of benzoxazine-based systems as a manner for inducing programmable properties into the final polybenzoxazines. **P. Froimowicz**

2:30 PMSE 183. Three-dimensional hierarchical porous carbons derived from polybenzoxazine and their applications in gas storage and supercapacitors. **T. Chaisuwan**, S. Wongkasemjit, N. Manmuanpom

3:00 PMSE 184. Advances in molecular modeling of benzoxazine based thermoset polymers. **T.J. Mustard**, J. Sanders, A. Browning, H. Kwak, C.M. Krauter, S. Christensen, M. Halls

3:30 Intermission.

3:45 PMSE 185. Benzoxazine studies with Gaussian simulation. **T. Heyl**, L. Han, D. Iguchi, P. Gil, V. Sedwick, C. Arza, S. Ohashi, D. Lacks, H. Ishida

4:05 PMSE 186. Understanding the vibrational structure, ring-opening kinetics of oxazine ring, hydrogen bonding system and smart *ortho*-structure molecular design of higher performance polybenzoxazines. **L. Han**, K. Zhang, P. Froimowicz, D. Iguchi, P. Gil, T. Heyl, V. Sedwick, M. Salum, C. Arza, S. Ohashi, D. Lacks, H. Ishida

4:25 PMSE 187. Cardanol as natural source of phenol for preparation of polybenzoxazines thermosets: Effect of the aliphatic side chain on the properties. **R. Ganfoud**, P. Verge, N. Guigo, L. Puchot, N. Sbirrazzuoli

4:45 PMSE 188. Three different approaches to reduce the polymerization temperature of benzoxazines. A. Martos, J. Salabert, M. Soto, K. Koschek, J. Marquet, **R.M. Sebastián**

Section E
New Orleans Marriott Canal Street
Studio 2

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Biofouling & Bioseparations

Cosponsored by DAC‡
Financially supported by North American Membrane Society
D. Bhattacharyya, I.C. Escobar, B.D. Freeman, C.M. Stafford, *Organizers*
Y. Ding, S. Wickramasinghe, *Presiding*

1:30 PMSE 189. Grafting zwitterions onto membrane surface using bioadhesive polydopamine to enhance antifouling properties for wastewater reuse. **H. Lin**, N. Shahkaramipour, C. Cheng

2:00 PMSE 190. Switchable zwitterionic membrane surface chemistry for biofouling control. **S.T. Weinman**, M. Bass, S. Pandit, V. Freger, M. Herzberg, S.M. Husson

2:30 PMSE 191. Novel block co-polymer that self-assembles to brush-like monolayer on varied surfaces and slows down biofilm formation. **Y. Kaufman**, C. Ziemba, M. Piatkovsky, D. Priftis, H. Acar, J. Mao, M. Benami, M.V. Tirrell, M. Herzberg

‡*Cooperative Cosponsorship*

3:00 Intermission.

3:30 PMSE 192. Surface characterization and chemical cleaning of reverse osmosis membranes from a full-scale water reuse facility: Role of silicates and biofouling on aging. **B. Abada**, S. Chellam

4:00 PMSE 193. High performance electrospun nanofiber membranes for protein purifications. S.R. Wickramasinghe, **X. Qian**, S. Chen

4:30 PMSE 194. Use of confocal microscopy and SEM to study virus capture behavior of Planova hollow fiber virus filters. **H. Nazem-Bokaee**, D. Chen, S.M. O'Donnell, A.L. Zydney

5:00 PMSE 195. Chitosan/hyaluronan coatings tailored for tumor cell adhesion: Influence of the topography and capacitance gradient. **J.M. Neto**, R.A. Bataglioli, S. Pimentel, H.F. De Carvalho, M.M. Beppu

Section F
New Orleans Marriott Canal Street
Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

1:30 PMSE 196. Theory and simulation of topological non-idealities in polymer networks. **B.D. Olsen**, J.A. Johnson, R. Wang, T. Lin

2:00 PMSE 197. Statistical and hydrodynamic properties of graph-shaped polymers and quaternions. **T. Deguchi**, E. Uehara

2:30 PMSE 198. Theory, simulation, and neutron scattering from cyclic polystyrene and exact linear analogs. **M.J. Hore**, S.M. Grayson, A. Jayaraman, F.M. Haque, T.E. Gartner

2:50 PMSE 199. Dilute solution properties of semiflexible ring polymers. **D. Ida**, T. Yoshizaki

3:10 Intermission.

3:20 PMSE 200. Entanglement in protein structures – knots, lassos and links: Applications in medicine. **J.I. Sulkowska**, P. Dabrowski-Tumanski, W. Niemyska

3:50 PMSE 201. Knot energy, complexity, and mobility of knotted polymers. **J.F. Douglas**, F. Vargas-Lara

4:20 PMSE 202. On chirality of molecular graphs. **K. Shimokawa**

4:50 PMSE 203. Computational studies of poly[*n*]catenanes. **P. Rauscher**, S.J. Rowan, J.J. De Pablo

Section G
New Orleans Marriott Canal Street
Studio 9

Clay-Polymer Composites: Nanoclays & Other Natural Nanoparticles

Clay Nanotubes & Nanofiber Composites

Financially supported by Applied Minerals, Inc.; Zibo Zhangdian Oriental Chemical Co., Ltd.
Y.M. Lvov, E. Ruiz-Hitzky, A. Takahara, L. Zhang, *Organizers*
N. Kotov, *Organizer, Presiding*

1:30 PMSE 204. Molecular aggregation states and physicochemical properties of (imogolite/polymer) hybrids. **A. Takahara**, Y. Higaki, W. Ma, L. Li

2:00 PMSE 205. Sepiolite-halloysite nanoarchitectures and their role in functional nanocomposites. **P. Aranda**, G. Lo Dico, L. Lisuzzo, B. Wicklein, G. del Real, G. Lazzara, E. Ruiz-Hitzky

2:30 PMSE 206. Biopolymer enhanced stabilization of tubular and flat sheet clays at the oil-water interface: Fundamentals, and applications to environmental remediation. **V.T. John**, O.G. Owoseni, Y. Su, M. Omarova

3:00 PMSE 207. Application of synthesized MOF@Halloysite nanotubes on gas adsorption capacity. **S. Lim**, D. Sohn

3:30 PMSE 208. Clay/hydrogel composites by gamma ray radiation. **D. Sohn**, J. Ryu, J. Kim

4:00 PMSE 209. Sepiolite-mediated transfer of nucleic acids in cells. **F.A. Castro Smirnov**, O. Piétrement, P. Aranda, E. Le Cam, B. Lopez, E. Ruiz-Hitzky

4:20 PMSE 210. Coarse grained force field for polymer clay nanocomposites. **P. Khan**, G. Goel

4:40 PMSE 211. Controlled loading and release of quercetin by natural halloysite nanotubes. **R. Li**, Y. Chen, X. Chen

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials

Frontal Polymerization

Sponsored by POLY, Cosponsored by PHYS and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
M. Becker, *Organizer*

8:00–10:00

11, 23, 66, 68, 124, 137-138, 145, 148, 150, 160-161, 191, 602. See previous listings.

223, 253, 258, 266, 270, 280, 288, 293, 305, 307, 312, 322, 327, 329, 336, 351-352, 357, 360, 372, 386, 399, 403, 407, 422, 424, 429, 437, 439, 442, 444, 464-465, 474, 488, 494, 542, 555, 562, 573, 578-580, 593. See subsequent listings.

TUESDAY MORNING

Section A
New Orleans Marriott Canal Street
La Galerie 6

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Novel Materials Design

Cosponsored by WCC
Financially supported by DuPont
Z. Bao, Y. Diao, G. Wang, *Organizers, Presiding*

8:30 Introductory Remarks.

8:40 PMSE 212. Block copolymers for high resolution patterning applications. **C.G. Willson**

9:10 PMSE 213. Development of scalable knittable functional polymer yarns. **S. Yang**

9:40 PMSE 214. Sustainable polymeric materials: Education, research and development, and commercialization. **M. Sabahi**, E. Reichmanis

10:10 Intermission.

10:25 PMSE 215. Making smart windows smarter. **Y. Loo**

10:55 PMSE 216. Si-containing polymers for nanoelectronics: From synthesis to applications in high-volume microchip manufacturing. **Q. Lin**

11:25 PMSE 217. Synthesis and phase behavior of highly functional block copolymers. **P. Gopalan**

Section B
New Orleans Marriott Canal Street
La Galerie 4

Symposium for Pan-American Science

Financially supported by ACS Brazil Chapter
B.D. Olsen, C. Ornelas, *Organizers*
E. Gomez, *Presiding*

8:30 PMSE 218. Phytoglycogen nanoparticles: Soft colloids from nature. **J. Dutcher**, M. Grossutti, H. Shamana, A. Maxwell, J. Atkinson

9:00 PMSE 219. Equilibrium and kinetic swelling in ultrathin films of phytoglycogen nanoparticles, hyaluronic acid and phytoglycogen:hyaluronic acid mixtures. **M. Grossutti**, K. Charlesworth, E. Bergmann, B. Baylis, J. Dutcher

9:20 PMSE 220. Withdrawn

9:40 PMSE 221. Use of lanolin on collagen films. **V. Martins**

10:00 Intermission.

10:20 PMSE 222. Can layer-by-layer be a good reservoir model for protein release? **L. Catalani**, M.C. Sogayar, A.F. Naves, G. Delechiave, A.C. Carreira, E. Kolanthai

10:50 PMSE 223. Plasma effects on barrier and solubility properties of protein films. **V.P. Romani**, V. Martins, B.D. Olsen, M. Collares, J. Oliveira

11:10 PMSE 224. Synthesis and characterization of lipopeptide nanostructures: application as catalysts for aldol reactions in aqueous medium. **W.A. Alves**

11:40 PMSE 225. Multiplex infrared spectroscopy imaging for monitoring spatially resolved redox chemistry. **F.N. Crespilho**

Section C
New Orleans Marriott Canal Street
Studio 3

Polymers with Complex Architecture: From Synthesis to Self-Assembly

Keynote Speaker Session

Financially supported by NSF, BASF, ExxonMobil, LG MMA, and Wyatt Technology, Department of Chemistry & Biochemistry at Florida State University
C.Y. Ryu, G. Stein, *Organizers*
J.G. Kennemur, M. Seo, *Organizers, Presiding*

8:30 PMSE 226. Withdrawn.

9:15 PMSE 227. Unique behaviors for molecular bottlebrush block polymers vs. linear analogs: Solution- vs. substrate-mediated assembly behaviors. **K.L. Wooley**

10:00 Intermission.

10:15 PMSE 228. Proton transport through lamellar water channels in chain-folded precisely sulfonated polyethylene. **K.I. Winey**

11:00 PMSE 229. Macromolecular metamorphosis: Stimulus-triggered topological transformations of polymer architecture. H. Sun, C.P. Kabb, Y. Dai, M. Hill, A. Bapat, **B.S. Sumerlin**

Section D
New Orleans Marriott Canal Street
La Galerie 5

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

P. Froimowicz, I. Hamerton, H. Ishida, *Organizers*
T. Chaisuwan, L. Han, *Presiding*

8:00 PMSE 230. Shape memory polymers based on polybenzoxazine alloys and composites enhancement of recovery stress and thermal properties. **S. Rimdusit**, M. Okhawilai, C. Jubsilp

8:35 PMSE 231. Smart latent catalyst containing o-trifluoroacetamide functional benzoxazine: Precursor for low temperature formation of very high performance polybenzoxazole with low dielectric constant and high thermal stability. K. Zhang, **L. Han**, P. Froimowicz, H. Ishida

8:55 PMSE 232. Synthesis of a bisbenzylidieneacetone/ bis(4-hydroxyphenyl) propanone -containing benzoxazine and its photo- and thermally-cured thermoset. **C. Lin**, Z. Chen, C. Chen, M. Wang

9:25 PMSE 233. Potential of poly(benzoxazine) as immobilization matrix for microbiosensors. J. Lin, S. Daboss, W. Schuhmann, **C. Kranz**

9:55 Intermission.

10:15 PMSE 234. Preparation and characterization of carbon fiber reinforced amide-co-imide functional polybenzoxazine and polybenzoxazole composites. **C. Ma**, L. Han, Z. Ma, X. Yin, H. Ishida

10:35 PMSE 235. Fiber reinforced polybenzoxazine: From benzoxazine chemistry to lightweight materials. **K. Koschek**, H. Schäfer, J. Werner, M. Soto

11:05 PMSE 236. Tribological and thermal properties of friction composites based on polybenzoxazine. **C. Jubsilp**, S. Rimdusit

11:35 PMSE 237. Benzoxazine-functionalized graphene oxide for synthesis of new nanocomposites. E.E. Biru, **S.A. Garea**, **H. Iovu**

Section E
New Orleans Marriott Canal Street
Studio 2

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

MOFs & 2D Membrane Materials

Cosponsored by DAC‡
Financially supported by North American Membrane Society

D. Bhattacharyya, I.C. Escobar, B.D. Freeman, *Organizers*
C.M. Stafford, *Organizer, Presiding*
J.A. Howarter, *Presiding*

8:15 Introductory Remarks.

8:20 PMSE 238. Synthesis of ultrathin metal-organic framework membranes for gas and ion separations. **H. Wang**

9:00 PMSE 239. Evaluating an open metal site MOF for mixed-matrix membranes. **Z.P. Smith**, J. Bachman, T. Li, B. Gludovatz, V. Kusuma, T. Xu, D.P. Hopkinson, R. Ritchie, J.R. Long

9:30 PMSE 240. Graphene oxide-based desalination membranes. **M.R. Hibbs**, C.D. Mowry, V. Pinon, K.R. Zavadil, A.S. Pimentel, C. Stewart, M.L. Gucik, L. Biedermann

10:00 Intermission.

10:30 PMSE 241. Facile grafting of ionic liquids onto halloysite nanotubes via an atom transfer radical polymerization method. **H. Zhang**, H. Song

11:00 PMSE 242. Graphane based membranes: Water transport. **X. Zhang**

11:30 Concluding Remarks.

Section F
New Orleans Marriott Canal Street
Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

8:30 PMSE 243. Synthesis and characterization commercially relevant cyclic polymers. Z. Miao, W. Niu, T. Kubo, K.C. Bentz, D.A. Savin, B.S. Sumerlin, **A.S. Veige**

9:00 PMSE 244. Macrocyclic conjugated polymers of novel topology. B.J. Lidster, S. Hirata, S. Matsuda, T. Yamamoto, V. Komanduri, D.R. Kumar, M. Vacha, Y. Tezuka, **M.L. Turner**

9:30 PMSE 245. Unusual cyclic polymerization through Suzuki-Miyaura coupling of polyarylene bearing diboronate at both ends with excess dibromoarylene. H. Sugita, Y. Ohta, **T. Yokozawa**

9:50 Intermission.

10:00 PMSE 246. Controlled ring-expansion cationic polymerization: Precise construction of ring-based architectures. **M. Ouchi**

10:30 PMSE 247. Progress towards the synthesis of jellyfish block-copolymers via REP/CRP. **Y.D. Getzler**, S.E. Wright, N. Gutsche, J. Bouquot, W. Cole, M. Itschner

10:50 PMSE 248. Cyclic polylactides via ring-expansion polymerization. H.R. Kricheldorf, F. Scheliga, **S.M. Weidner**

11:20 PMSE 249. Simple and versatile approach to cyclic polymers via lactam mediated ring-opening polymerization of cyclic monomers. C. Shi, F. Du, **Z. Li**

Section G
New Orleans Marriott Canal Street
Studio 9

Clay-Polymer Composites: Nanoclays & Other Natural Nanoparticles

Polymer-Nanoparticle Composites

Financially supported by Applied Minerals, Inc.; Zibo Zhangdian Oriental Chemical Co., Ltd.

N. Kotov, Y.M. Lvov, E. Ruiz-Hitzky, A. Takahara, L. Zhang, *Organizers*
B. Guo, *Presiding*

8:00 PMSE 250. Nanocomposite-based flexible lithium ion batteries for wearable sensor applications. **M. Agarwal**, N. Aliahmad

8:30 PMSE 251. Brick-and-mortar biocomposites from cellulose nanofibrils and clay nanoplatelets. **L. Medina**, L. Berglund

9:00 PMSE 252. Cellulose nanocrystals as renewable nanofillers for polymeric (nano)composites. **J. Raquez**

9:30 PMSE 253. Incorporation of cellulose nanocrystals into poly(ethylene) matrix by polymerization filling. **K.D. Hendren**, P.A. Deck, J. Foster, T.W. Baughman

10:00 Intermission.

10:10 PMSE 254. Loading of indocyanine green within polydopamine-coated laponite nanodisks for targeted cancer photothermal and photodynamic therapy. F. Xu, X. Li, M. Liu, Z. Xiong, **X. Shi**, R. Guo

10:40 PMSE 255. Interfacial effect on crystallization behavior of polyethylene/ silica composites. **D. Wang**, W. Zhao, Y. Su

11:10 PMSE 256. Dual mode image nanoprobes used for MR-NIRF imaging. **C. Bai**, Y. Zhang

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, ENVR‡, INOR, PMSE‡ and PRES‡

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
Sponsored by POLY, Cosponsored by BIOT, MEDI and PMSE

Undergraduate Research in Polymer Science
Sponsored by POLY, Cosponsored by CHED and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY AFTERNOON

Section A
New Orleans Marriott Canal Street
La Galerie 6

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Advanced Structure Analysis

‡*Cooperative Cosponsorship*

Cosponsored by WCC
Financially supported by DuPont
Z. Bao, Y. Diao, G. Wang, *Organizers, Presiding*

1:30 PMSE 257. Benefit of a multiscale approach for the investigation of energy storage materials. **E.S. Takeuchi**, A.C. Marschilok, K.J. Takeuchi

2:00 PMSE 258. Smart gel-based materials from design to application via organic-inorganic hybrid technology. **M. Zhu**

2:30 PMSE 259. Twisted structures in lyotropic chromonic liquid crystals: Here, there and everywhere. **M. Srinivasarao**, J. Park, K. Nayani, J. Fu, R. Chang

3:00 Intermission.

3:15 PMSE 260. Polymeric bioactives: Polymers from bioactives and as bioactives. **K.E. Uhrich**

3:45 PMSE 261. Low-hanging fruit for machine learning in materials science: Imaging. **N. Persson**, M. McBride, M. Grover, E. Reichmanis

4:15 PMSE 262. Review of the hiring and promotion of female faculty members at nine prestigeous chemistry departments. **V.J. Kuck**

4:45 PMSE 263. Controlled assembly of poly(3-hexylthiophene): From fundamental understanding of conjugated polymer assembly process towards stretchable electronics. **D. Choi**, S. Lee, E. Reichmanis

Section B
New Orleans Marriott Canal Street
La Galerie 4

Symposium for Pan-American Science

Financially supported by ACS Brazil Chapter
C. Ornelas, *Organizer*
B.D. Olsen, *Organizer, Presiding*

1:30 PMSE 264. Development of new well-defined multifunctional dendrimers for nanomedicine applications. **C. Ornelas**, D. Bertuzzi, M. Ramos Jr, C. Braga, T. Becher, A. Porras, D. Souto

2:00 PMSE 265. Nanocomposites applied as photohyperthermia agents: Cancer therapy and toxicity studies. **V. Zucolotto**

2:30 PMSE 266. Fluorescent proteins as emission sensitizing agents in europium nanoparticles bioconjugates. **F.E. Maturi**, C.E. Mills, S.J. Ribeiro, B.D. Olsen

2:50 PMSE 267. Development of new template strategies for the synthesis of polyrotaxanes. A.F. Alcantara, L. Fontana, V. Rigolin, **J.D. Megiatto**

3:10 Intermission.

3:30 PMSE 268. Role of fast polymer dynamics as quantified by inelastic neutron scattering on the mechanical toughness on polymeric materials. **C.L. Soles**

4:00 PMSE 269. Recent instrumentation advances offer new opportunities in electron microscopy of polymers. **E. Gomez**

4:30 PMSE 270. Poly (butylene succinate): Applications from the farm to the health. **F. Gomes Souza Jr**

5:00 PMSE 271. Novel hybrid polymeric adsorbents for wastewater treatment. **P.V. Toledo**, D.P. Limeira, **D. Petri**

Section C
New Orleans Marriott Canal Street
Studio 3

Polymers with Complex Architecture: From Synthesis to Self-Assembly

Financially supported by NSF, BASF, ExxonMobil, LG MMA, and Wyatt Technology, Department of Chemistry & Biochemistry at Florida State University
J.G. Kennemur, C.Y. Ryu, M. Seo, G. Stein, *Organizers*
H. Chung, *Presiding*

1:30 PMSE 272. Tapered (cone-shaped) polymers by sequential-addition of macromonomers ring-opening metathesis polymerization (SAM-ROMP). **J.B. Matson**, J. Foster, S. Radzinski

2:00 PMSE 273. Stimuli-responsive porous materials by tailoring hybrid-polymer core-shell architectures. **S. Vowinkel**, T. Winter, A. Schlander, M. Gallei

2:20 PMSE 274. Probing structure of temperature-responsive polymersomes assembled from ABA triblock copolymers. **Y. Yang**, A. Alford, V.A. Kozlovskaya, L. He, V. Urban, E.P. Kharlampieva

2:40 PMSE 275. Dynamics of PS_2-PI_2 miktoarm polymers in geometrical confinement. **E. Mapesa**, T. Kinsey, J. Sangoro

3:00 Intermission.

3:15 PMSE 276. Low strain, more gain: Harnessing polypentenamers towards complex precision architectures. **J.G. Kennemur**, W.J. Neary, S. Brits, G. Palui, A. Kendrick

3:45 PMSE 277. *In situ* self-assembly study in bio-based thin films. **C. Brett**, N. Mittal, W. Ohm, D. Soderberg, S. Roth

4:05 PMSE 278. Structure formation of block copolymer based photonic materials and functionalization strategies. **M. Appold**, M. Gallei

4:25 PMSE 279. Supramacromolecular strategy for overcoming antibiotic resistance. **X. Li**, A. Delawder, T. Kincaid, R. Li, A.F. Greene, J.R. Chartock, J.C. Barnes

4:45 PMSE 280. Singlet oxygen degradable micelles for delivery of anticancer drugs. **V. Brega**, S.W. Thomas

Section D
New Orleans Marriott Canal Street
La Galerie 5

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

P. Froimowicz, I. Hamerton, H. Ishida, *Organizers*
S. Chirachanchai, B. Kiskan, *Presiding*

1:30 PMSE 281. Study on the weight loss of benzoxazine during the curing process. **Q. Ran**, Y. Gu

2:00 PMSE 282. Alternative routes for the development of benzoxazine resins: A green and sustainable approach. **D. Lomonaco**

2:30 PMSE 283. Withdrawn

3:00 PMSE 284. Structural tuning of polybenzoxazine/epoxy composites with dual crosslinking network for corrosion protection. **C. Zhou**, Z. Xin

3:20 Intermission.

3:40 PMSE 285. Superhydrophobic coatings and separators: Polybenzoxazine nanocomposites. **R.C. Advincula**

4:00 PMSE 286. Polybenzoxazines/POMS composites: Preparation and properties. **R. Xu**, D. Yu

4:20 PMSE 287. High-performance copolymers derived from fully bio-based benzoxazine monomers. **J.R. Oliveira**, L.R. Kotzebue, A. Sales, S.E. Mazzetto, D. Lomonaco

4:40 PMSE 288. Novel glass fabric reinforced polybenzoxazine-silicate composites along with polyvinyl butyral for high service temperature applications. **R. Sriperambudur**

5:00 PMSE 289. Preparation of flexible shape memory polybenzoxazine through chemical structure manipulation and hydrogen bonds control. **S. Zhang**

Section E
New Orleans Marriott Canal Street
Studio 2

Cooperative Research Award: Symposium in honor of D. Bruce Chase & John F. Rabolt

Financially supported by University of Delaware, Department of Materials Science & Engineering
S.C. Jana, D.C. Martin, *Organizers, Presiding*

1:00 PMSE 290. Photomobility and orientation in azomaterials. **C. Pellerin**, A. Laventure, J. Vapaavuori, R. Sabat, O. Lebel

1:30 PMSE 291. Vibrational spectroscopy and two-dimensional correlation analysis of bioplastics. **I. Noda**, B. Chase, J.F. Rabolt

2:00 PMSE 292. End-of-shift measurement of airborne β-quartz and diesel particulate matter by mid-infrared diffuse transflection spectrometry. D. Parks, A. Miller, **P.R. Griffiths**

2:30 PMSE 293. AFM-IR studies of individual electrospun nanofibers of bio-based poly[(R)-3-hydroxybutyrate-*co*-(R)-3-hydroxyhexanoate] (PHBHx). **L. Gong**, B. Chase, I. Noda, C.A. Marcott, J.F. Rabolt

3:00 Intermission.

3:30 PMSE 294. Structure and properties of oriented polymer nanofibers. **D.C. Martin**, V. Subramanian, J. Liu, S. Chhatre, B.S. Shim

4:00 PMSE 295. Overcoming the infrared diffraction limit: Submicron spatial resolution IR spectroscopy using a non-contact optical method. **C.A. Marcott**, E. Dillon, S. Zayats, K. Kjoller, C. Prater

4:30 PMSE 296. Characterization of metastable crystalline polymorphs in electrospun polymer nanofibers using AFM-IR, XRD and selected area electron diffraction (SAED). **J.F. Rabolt**, B. Chase

Section F
New Orleans Marriott Canal Street
Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

1:30 PMSE 297. Purification and characterization of cyclic polymers. **T. Chang**

2:00 PMSE 298. Separation of cyclic and linear polymers based on selective intercalation into graphite oxide. **F. Barroso-Bujans**, A. Alegria

2:30 PMSE 299. Comparison of critical adsorption points of ring polymers with linear polymers. **Y. Wang**, T. Chang

2:50 Intermission.

3:00 PMSE 300. Pore translocation of knotted DNA. A. Suma, **C. Micheletti**

3:30 PMSE 301. Tandem mass spectrometry approaches for determining polymer structure, sequence, and topology. **C. Wesdemiotis**

4:00 PMSE 302. Single-molecule characterization of topological polymer dynamics. **S. Habuchi**

4:30 PMSE 303. Synthesis and photophysical studies of cyclic poly(p-phenylenevinylene)s by ring-expansion metathesis polymerization of strained 1,9-paracyclophanedienes. B. Lidster, S. Hirata, S. Matsuda, T. Yamamoto, **V. Komanduri**, D.R. Kumar, Y. Tezuka, M. Vacha, M.L. Turner

Section G
New Orleans Marriott Canal Street
Studio 9

Additive Manufacturing of Structures & Functional Devices: Materials, Methods, Models & Testing

Biomaterials & Regenerative Medicine

J. Lewis, C.R. Snyder, *Organizers*
D. Berrigan, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 PMSE 304. Development of resorbable polymer inks for cDLP printing and their use in regnerative medicine. **M. Becker**

2:05 PMSE 305. 3D printed organ models with physical properties of tissue and integrated sensors. **K. Qiu**, M.C. McAlpine

2:25 PMSE 306. Effect of drugs as fillers on the 3D print quality and degradation of a soft amorphous polyester. **A. Joy**, T.

‡*Cooperative Cosponsorship*

Jain, I. Isayeva

2:45 PMSE 307. Biodegradable, 3D-printable PEG-PPF hydrogels for tissue repair. **R. Dilla**, J. Wilson, M. Becker

3:05 Intermission.

3:20 PMSE 308. 3D printing of liquid and soft materials: Applications from regenerative medicine to wearable sensing. T. Hinton, A. Lee, A. Hudson, S. Abdollahi, **A.W. Feinberg**

3:50 PMSE 309. Self-assembled 3D-printed Janus scaffolds for the regeneration of interfacial tissues. **S. Camarero-Espinosa**, C. van Blitterswijk

4:10 PMSE 310. Chitosan-pluronic diacrylate hydrogels as 3D printable material for heavy metal ion adsorption. **G. Adikari Appuhamillage**, D.R. Berry, C.E. Benjamin, M.A. Luzuriaga, J.J. Gassensmith, R.A. Smaldone

4:30 PMSE 311. Fabrication of self-cleaning antireflective polymer surfaces by mimicking underside leaf hierarchical surface structures. **S. Mattaparthi**, C. Sharma

4:50 PMSE 312. Low viscosity plant based building blocks for additive manufacturing. **J. Vergara**, K. Pauperowicz, D. Bolarin, S.K. Yadav, J.J. La Scala, G. Palmese

GSSPC: Finding Our Place at the Bottom

Symposium in honor of Richard Feynman

Sponsored by CHED, Cosponsored by ANYL‡, COLL‡, INOR, PHYS‡, PMSE‡ and PRES‡

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
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Polymer Networks: Soft Gels to Stiff Networks
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Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

TUESDAY EVENING

Section A
Ernest N. Morial Convention Center Hall D

Joint PMSE-POLY Poster Session

Clay-Polymer Composites: Nanoclay & Other Natural Nanoparticles

Cosponsored by POLY
M. Becker, *Organizer*

6:00–8:00

PMSE 313. One-step preparation of electrically conductive polyurethane composite by self-assembly of two-dimensional material. **F. Chen**, D.H. Adamson

PMSE 314. Conductive polymer composites from self-assembled graphene networks by photo and microwave induced polymerization. **T. Hui**, D.H. Adamson

PMSE 315. MoS_2 dispersed epoxy composite: Influence of solvent quality and surface chemistry to local chemical network formation and its influence on nanoscale toughening mechanism. **D. Nepal**, J. Ryan, I. Barrett, R. Wheeler, I.E. Pavel Sizemore, G.S. Kedziora, S. Roy, J. Moller, A. Sharits

PMSE 316. Clay nanotube self-assembly on hair surfaces: Formulation for medical and hair color treatments. **A. Panchal**, R. Fakhrullin, Y.M. Lvov

PMSE 317. Bacterial proliferation on clay nanotube Pickering emulsions for oil spill bioremediation. **A. Panchal**, L. Swientoniewski, Y.M. Lvov, T. Yu, D. Zhang, M. Omarova, G. Fakhrullina, V.T. John, D.A. Blake

PMSE 318. Self-assembly of halloysite nanotubes in microchannels for functionalizing microfluidic devices to capture cells. **M. Pickett**, A. Panchal, N.D. Crews, Y.M. Lvov

PMSE 319. Preparation and characterization of exfoliated mica-polyamide 66 nanocomposites using high shear melt processing. **A. Tewatia**, J. Lynch-Branzoi

PMSE 320. Beyond percolation: Exploring the effects of high graphene loading on polymer-graphene composites and *in situ* bulk polymerizations. **S. Ward**, D.H. Adamson

PMSE 321. Synthesis and investigation of amphiphilic polypeptoid- functionalized halloysites nanotubes (HNTs) as stabilizer towards oil spill remediation. **T. Yu**, D. Zhang, L.T. Swientoniewski, D.A. Blake, M. Omarova, V.T. John, A. Panchal, Y.M. Lvov

Section A
Ernest N. Morial Convention Center Hall D

Joint PMSE-POLY Poster Session

General Posters: New Concepts in Polymeric Materials

Cosponsored by POLY
M. Becker, *Organizer*

6:00–8:00

PMSE 322. Acrylic-polyurethane based graft-interpenetrating polymer networks. **N. Alizadeh**, V. Agrawal, A. Celestine, M. Auad

PMSE 323. Surface immobilization of poly(*N*-isopropylacrylamide) on polycarbonate by inter-diffusion and basic thermodynamic interactions. **M. Alyami**, B.M. Zhang Newby, A. Alghunaim, E.T. Brink

PMSE 324. Cyanotriphenylamine-based polyimidothioethers as multifunctional materials for fluorescent electrospun fibers, electrochromic, and electrofluorochromic devices. **H. Yen**, C. Chang, G. Liou

PMSE 325. Thermotropic liquid crystalline oligomers with selectively removable moieties for nanofabrication. **M. Aoki**, K. Shimokawa, Y. Nabae, T. Hayakawa

PMSE 326. Ultra-high molecular weight block copolymers for photonic applications in the bulk state. **M. Appold**, L. Proskurjakov, M. Gallei, E. Grune, H. Frey

PMSE 327. Phosphate modified graphene oxide as a mechanically sound, water stable biomaterial capable of controlled release. **A. Arnold**, B. Holt, S.A. Sydlik

PMSE 328. Synthesis and application of polyelectrolyte with super acid group (III): Influence of proton conductivity and gas permeability on PEFC performance. **M. Asano**, M. Fujita, Y. Takeoka, M. Rikukawa

PMSE 329. Infrared actuation-induced simultaneous reconfiguration of surface color and morphology for smart artificial skins. **S. Banisadr**, J. Chen

PMSE 330. Polymeric ionic liquids: Synthetic challenges and lubricant applications. **A. Bapat**, L. Cosimbescu, R. Erck, N. Demas

PMSE 331. Synthesis and characterization of self-assembling ABC triblock co-polypeptides. **B. Barnes**, L. Stein, C. Machado, I. Smith, D.A. Savin

PMSE 332. Structure and drug release properties of layer-by-layer thin films controlled by pH and drug loading strategies. **R.A. Bataglioli**, M.M. Beppu

PMSE 333. Systematic study on effect of raster solvent vapor annealing using dual solvents on morphology of block copolymers under thin film confinement. **S. Behzadinasab**, S. Chatterjee, B. Lwoya, M. Uddin, J.N. Albert

PMSE 334. Thermal and rheological response of metallized PVDF/PMMA composites with nanoscale and microscale aluminum. **J. Bencomo**, J. McCollum, S.T. Iacono

PMSE 335. Thin film stability in linear and cyclic blends of poly(β-caprolactone) (PCL). **A. Bergeson**, G. Kelly, F.M. Haque, S.M. Grayson, J.N. Albert

PMSE 336. Thermally reversible Diels-Alder soft polymers for 3D printing. **D.R. Berry**, R.A. Smaldone

PMSE 337. Withdrawn.

PMSE 338. Synthesis and characterization of low density polymer/graphene nanocomposite foams. **E. Brown**, D.H. Adamson

PMSE 339. Pegylated polybenzoxazine networks with increased thermal stability from miscible blends of tosylated poly(ethylene glycol) and a benzoxazine monomer. **E.A. Brown**, D.A. Rider

PMSE 340. Pyrrole containing semiconducting small molecules and polymers for organic electronics. **C. Bulumulla**, R. Kularatne, R. Gunawardhana, H. Nguyen, M.C. Biewer, M.C. Stefan

PMSE 341. Reactively blended wheat gluten gels loaded with high molecular weight polyethylene oxide. **J. Caffyn**, R. Mehta, R. Parnas

PMSE 342. Structural characterization of organotin polymers from the antiviral lamivudine and dipeptide diglycine. **C.E. Carraher**, P. Slawek, F. Mosca, M.R. Roner, J.E. Haky

PMSE 343. Synthesis of Group IVB and organotin-containing polyamine esters, polyethers, and polyesters. **C.E. Carraher**, M.R. Roner, E. StFort, N. Ezzell, J. Frank, D. Patel, J.D. Einkauf, F. Russell, A. Moric-Johnson, L.C. Miller, E. Quiles, Z. Rabinewitz, E. Mittelmark

PMSE 344. Exposure predictions for rapid risk assessment of phase-separated additives in medical device polymers. **V. Chandrasekar**, A. Hood, A. Bajaj, T.V. Duncan, J. Zheng, B. Casey, D. Saylor

PMSE 345. Self-assembly of PS-b-PVMS and thiol-modified PS-b-PVMS thin films under various annealing conditions. **S. Chatterjee**, B. Lwoya, J.N. Albert

PMSE 346. Synthesis and properties of oligo(2,6-dimethyl phenylene oxide) s-containing polybenzoxazine with a characteristic of low dissipation factor. C. Lin, K. Lee, **C. Chen**

PMSE 347. Soluble porous organic polymer by imine condensation. **N. Chen**, S. Dai

PMSE 348. Photopatterned polyelectrolyte complexes as shape-directing templates for thermoreversible biopolymer gels. **K. Choudhuri**, U.K. de Silva, Y. Lapitsky

PMSE 349. Withdrawn.

PMSE 350. Sequence-defined metal templation as a strategy for the synthesis of functional materials. **N.D. Colley**, A.F. Greene, J. Fisher, X. Li, J.C. Barnes

PMSE 351. Enhanced ion transport in disordered block copolymers of ammonium-based polymerized ionic liquids. M. Harris, M.F. Heres, **J. Coote**, G. Stein, J. Sangoro

PMSE 352. Controlling the morphology of polyacrylonitrile based carbon fiber precursors by molecular design. **K. Cordell**, J.S. Wiggins

PMSE 353. Architectural core-shell metal catalyst synthesis onto/into clay nanotubes. **Y.A. Darrat**, A. Stavitskaya, V. Vinokurov, C. Colletti, J. McDonald, Y. Lvov

PMSE 354. Halloysite nanotube composites for enhancing lithium-sulfur battery efficiency. **Y.A. Darrat**, Y. Pei, Y. Wang, M. Norwood, Y.M. Lvov, S. Wang

PMSE 355. Connecting block copolymers with scissile mechanophores. **B. Davis**, Y.C. Simon

PMSE 356. Effects of regiochemistry on the properties and gas separation performances of ionic polyimides. **G.P. Dennis**, K.E. O'Harra, J.W. Whitley, E.M. Jackson, **J.E. Bara**

‡*Cooperative Cosponsorship*

PMSE 357. Synthesis and characterization of PEG-poly(propylene fumarate) hydrogels. **R. Dilla**, J. Wilson, M. Becker

PMSE 358. Molecular scale insight into poly(ethylene oxide)/cyclodextrin-based polyrotaxanes. **M. Ebrahiminia**, **D. Dong**, D. Bedrov

PMSE 359. Investigation on the fabrication of a superhydrophobic surface on solar panels. **P.E. Engen**, L. Dong, M. Scholten, R.S. Majerle

PMSE 360. Vapor-phase polymerization of poly(3,4-ethylenedioxythiophene) (PEDOT)/TiO2 and PEDOT/TiO2/ graphene composite fibers as electrode materials for supercapacitors. **M.T. Fox**, L. Tong, W.E. Jones, W.E. Bernier

PMSE 361. Withdrawn.

PMSE 362. Co, Fe, Cu catalysts supported on halloysite nanotubes for partial oxidation of aromatic compounds. **A.P. Glotov**, Y. Chudakov, A. Maria, A. Stavitskaya, E. Smirnova, E. Ivanov, V. Vinokurov, Y.M. Lvov

PMSE 363. Dissipative particle dynamic (DPD) simulations to predict self-assembly behavior of ternary block copolymer-homopolymer blends. **A. Goodson**, G. Liu, A.S. Raymond, M.S. Rick, H. Ashbaugh, J.N. Albert

PMSE 364. VO_2@SiO_2/PNIPAm thermochromic hybrid nanomaterials for smart window. Y. Wang, Y. Gao, L. Li, **X. Guo**

PMSE 365. Synthesis and properties of chiral hexa-*peri*-hexabenzocoronenes. **K. Hamal**

PMSE 366. Exploring "click" chemistry to synthesize and characterize cyclic polyethers. **F.M. Haque**, S.M. Grayson

PMSE 367. Sequential nucleophilic click reaction for functional degradable polymers: Design, synthesis and application. **H. He**, S. Thayumanavan

PMSE 368. Fabrication and application of micro-patterned PDMS composite membranes in pervaporation process for ethanol recovery from aqueous solution. **X. He**, T. Wang, J. Chen, J. Li

PMSE 369. Melt-processable and nanostructured polyethylene reactor blends entering a new range of mechanical performance and wear resistance. **T. Hees**, R. Mülhaupt

PMSE 370. Degradable polymers with antioxidant pendent groups. **L.J. Hill**, C. Jaconette, C. Warlick, H. Sims, B. Hinkley

PMSE 371. Synthesis and electrochemical properties of polybenzoxazine-derived nanoporous carbon electrode materials for supercapacitors. **P. Hiranpattanakul**, S. Wongkasemjit, T. Chaisuwan

PMSE 372. Synthesis, characterization, and evaluation of non-nucleophilic dispersants for automotive applications. **T. Holbrook**, G. Masson, R.F. Storey

PMSE 373. Synthesis and characterization of a novel β-cyclodextrin modified polyacrylamide and its rheological properties in aqueous solutions by hybriding with silica nanoparticles. **X. Hu**, Y. Ke

PMSE 374. Synthesis and catalytic reaction activity of gold nanoparticles/ diblock ionomers (V): Effect of molecular weight. **H. Inoue**, M. Fujita, Y. Takeoka, M. Rikukawa

PMSE 375. Synthesis and evaluation of polybetaine-type ion gel electrolyte(II) effect of zwitterionic unit on Li-ion conductivity. **J. Ishii**, Y. Takeoka, M. Rikukawa, M. Fujita

PMSE 376. Effects of the addition of relatively low MW acidic copolymers on the dispersion of asphaltenes in heavy crude oil. **M. Jo**, H. Lee, **J. Kim**

PMSE 377. Thermal-healing behavior of sulfonated polystyrene ionomers neutralized with amines. **M. Jo**, H. Lee, **J. Kim**

PMSE 378. Vapor-printed polymers for enhanced solar cell efficiency and lifetime. **W. Jo**, V. Bulovic, K. Gleason

PMSE 379. Synthesis, mechanical, and structural properties of piezoelectric polyvinylidene fluoride doped with barium titanate nanoparticles. **A. Joaquim**, O. Paul, R. Turner, R. Parthasarathy, L. Ouyang, Y. Barnakov, F. Williams

PMSE 380. Compatibilization of polyester/polyamide blends: Phosphonated polyester ionomer as minor-component compatibilizer with divalent anion. **L. Ju**, J.M. Dennis, K.A. Valentine, T.E. Long, R.B. Moore

PMSE 381. Designing nanoporous carbon as adsorbents for CH_4 storage. **N. Kaewaramsri**, S. Wongkasemjit, T. Chaisuwan

PMSE 382. Withdrawn

PMSE 383. Exploring solution size changes of dendritic and linear equivalent polymers in a range of solvents. **O. Kareem**, S.M. Grayson

PMSE 384. Cross-linkable multi-stimuli-responsive hydrogel inks for direct-write 3D printing. **D. Karis**

PMSE 385. Propylene/propane separation using efficient carbon membranes derived from polyimide precursors. **C. Karunaweera**, S. Panangala, I.H. Musselman, K.J. Balkus, J.P. Ferraris

PMSE 386. Synthesis of tailored amphiphilic graft polymers with a tunable void volume for encapsulation. **C.B. Keller**, M. Ejaz, S.M. Grayson

PMSE 387. Fabrication of polyaniline/ MoS_2 nanocomposite with increased electrical conductivity for electrochemical capacitors. **Y. Kim**, J. Jang

PMSE 388. Synthesis and characterization of cardanol based vinyl ester resins as cross-linker units. **E. Kinaci**, E. Can, J. La Scala, G.R. Palmese

PMSE 389. Synthesis and biosensing properties of polythiophene having phosphonium group (III): Interaction with DNA. **F. Kiyoshiro**, M. Fujita, Y. Takeoka, M. Rikukawa

PMSE 390. Synthesis of fluorine-containing block copolymers for porous membrane preparation via RAFT. **S. Kurimoto**, R. Nakatani, A. Chandra, Y. Nabae, T. Hayakawa

PMSE 391. Synthesis and assembly of (A-*branch*-B)$_n$ Janus bottlebrush polymers with ultra-small domain size. **A.N. Le**, Z. Guo, M. Zhong

PMSE 392. Patchy micelles of diblock copolymers as nanoscale building blocks for supracolloidal chains. **K. LEE**, D. Kang, J. Jeon, K. Kim, S. Jang, H. Kang, B. Sohn

PMSE 393. Antifragile interfaces between dental restorative materials and teeth. **S. Leguizamon**, T.F. Scott

PMSE 394. Synthesis and properties of unsymmetrical phosphinated benzoxazines. C. Lin, **C. Lin**, C. Chen

PMSE 395. Importance of evaluating dynamic encapsulation stability of amphiphilic assemblies in serum. **B. Liu**, S. Thayumanavan

PMSE 396. Self-assembly behavior of telechelic polymers with high-dipole moment chain ends. **C.H. Liu**, Y.C. Simon

PMSE 397. Conductivity measurement of PEO-LiFSI with co-polymer of PAA and tartaric acid. X. Li, **Y. Liu**, Y. Min

PMSE 398. Chemical crosslinked EVOH nanofiber aerogels with superelasticity and superoleophilicity for removal of oils and organic solvents. **J. Lu**, **R. Xiao**

PMSE 399. Low cost 3D printed microneedles for transdermal drug delivery. **M.A. Luzuriaga**, D.R. Berry, J.C. Reagan, R.A. Smaldone, J.J. Gassensmith

PMSE 400. Nanoporous thin films for use in oil/water separation. **B. Lwoya**, M. Uddin, S. Behzadinasab, S. Chatterjee, J.N. Albert

PMSE 401. Nanoporous materials with sub-10 nm pores prepared from a rod-coil diblock copolymer. **X. Lyu**, Z. Shen

PMSE 402. Synthesis of highly pH-responsive engineered sugar coated nanoscopic assemblies for biomedical application. **S. Maiti**, R. Bettinge, C. Cogswell, W. Du

PMSE 403. Solid state sensing of non-polar VOCs using the bistable expansion and contraction of helical polycarbodiimides. **N.R. Mammoottil**, J.F. Reuther, R. Campos, B.M. Novak

PMSE 404. Anti-inflammatory effect of drug-eluting electrospun polyisobutylene-based thermoplastic elastomeric fiber mat. **A.T. McClain**, A. Jindal, N.D. Leipzig, J.E. Puskas

PMSE 405. Intermolecular interaction of polymer brushes containing phosphorylcholine (PC) and inverse-PC. **S. Mihara**, M. Kobayashi

PMSE 406. Modular 3D-printing-enabled platform for the fabrication of living-composite models of human vasculature. **S.C. Millik**, A. Dostie, P. Smith, R. Shafranek, A. Saha, X. Su, A.B. Theberge, A. Nelson

PMSE 407. Fabrication of organogels containing fixed and mobile micelles. **K. Mineart**, W. Walker

PMSE 408. Effects of peptide backbone modification on the assembly, structure, and properties of chiral gold nanoparticle single helices. **S. Mokashi Punekar**, C. Liu, A. Merg, N.L. Rosi

PMSE 409. Synthesis of poly(phenylene) and poly(thiophene)-based block copolymer ionomers and their characterization. **Y. Nakano**, M. Fujita, Y. Takeoka, M. Rikukawa

PMSE 410. Carefully controlled poly(lactic acid) networks through "thiol-ene" cross-linking of β,β ene functionalized PLA polymers and multi-armed thiols. **B. Nicholas**, R.G. Toomey, N. Gallant

PMSE 411. Theoretical and experimental approach to predict the formation of crystalline covalent organic frameworks. **G. Occhialini**, S.O. Nielsen, R. Smaldone

PMSE 412. Insight into the anionic ring-opening polymerization with tetrabutylammonium azide to produce cyclic polyethers. **J. Ochs**, A. Veloso, F. Barroso-Bujans

PMSE 413. Ultrasensitive and selective non-enzymatic FET-type dopamine sensor based on organic conducting materials. **J. Oh**, J. Jang

PMSE 414. Adsorption behavior of quaternary-ammonium-containing block copolymer for boron nitride. **T. Okado**

PMSE 415. Effects of salts and pH on hydrolytic degradation of poly(L-lactic acid) blends. **H.T. Oyama**, M. Kimura, Y. Nakamura, R. Ogawa

PMSE 416. Preparation and self-assembly of liquid crystalline block copolymers constructed through hydrogen bonding. **H. Pan**, **Z. Shen**

PMSE 417. Conjugated polymer nano-ellipsoids assembled with octanoic acid and their polyurethane nanocomposites with simultaneous thermal storage and antibacterial activity. **J. Park**, D. Lee, K. Oh

PMSE 418. Hybrid diamine alloys for increased processability. **M. Patterson**, J.S. Wiggins

PMSE 419. Investigation of self-assembly of supramolecular host/guest polymer complexes in water utilizing simultaneous multiple sample lights scattering (SMSLS). **M.E. Payne**, C.W. Jarand, W.F. Reed, S.M. Grayson

PMSE 420. Release study for electrospun drug-loaded alginate- and chitosan-based nanofibers for modern wound dressings. **K. Penton**, W. Weeks, T. Brown, Z.K. Kinler, S. Hamilton

PMSE 421. Solvent free adhesive polymers synthesized using garlic extract components and elemental sulfur. **C. Perez**, K. Kamp, C. Jenkins

PMSE 422. Efficient synthesis of polyamino acid polymers. **E. Ponnusamy**, S. Rana

PMSE 423. Synthesis of lithium-ion-conducting solid polymer electrolyte membranes for energy-related applications. **B. Prasad Thapaliya**, C. Do-Thanh, H. Lyu, X. Sun, S. Dai

‡*Cooperative Cosponsorship*

PMSE 424. Edge charge neutralization of clay for improved nanocoating gas barrier. **S. Qin**, Y. Song, D. Hagen, J.C. Grunlan

PMSE 425. Withdrawn

PMSE 426. Investigating dendrimer kinetics via the synthesis of bis-MPA branched polymers. **M. Redding**, S.M. Grayson, O. Kareem

PMSE 427. Flow induced crystallization in isotactic polypropylene via simultaneous measurements of modulus, helicity and morphology. **D. Roy**, K. Migler

PMSE 428. New strategies for brush block copolymer synthesis and their application in polymer-based photonic crystals . **M.D. Ryan**, G. Miyake

PMSE 429. Microgels from xanthan gum and locust bean gum for potential biomedical applications. **S. Sagbas**, C. Silan, N. Sahiner

PMSE 430. Synthesis and evaluation of diblock polyelectrolytes (IV): Influence of side chains to glass transition temperature and proton transport properties. **I. Sakamoto**, M. Fujita, Y. Takeoka, M. Rikukawa

PMSE 431. Modeling of PVDF-alumina composites; atomistic simulations for predicting material properties. **F. Saleem**, J. McCollum, B. Runnels, S.T. Iacono

PMSE 432. P-doping poly(3-hexylthiophene) with F4TCNQ in binary solvent mixtures. **M. Sapolsky**, L. Freeman, P. Miller, D.S. Boucher

PMSE 433. Effects of the type of cations on the mechanical properties of ethyl acrylate ionomers thermally healed at room temperature. **I. So**, M. Jo, **J. Kim**

PMSE 434. Synthesis and modification of the surface of copper nanoparticles. N.R. Lima, **F.G. Souza JR**, B. Britto

PMSE 435. Fabricaion of nanoporous carbon as an anode for high power lithium-ion battery. **P. Sriboonpeng**, S. Wongkasemjit, T. Chaisuwan

PMSE 436. Amplification and optical reporting of interfacial molecular events using liquid crystals. **U. Sridhar**, K. Iwabata, N.L. Abbott, S. Thayumanavan

PMSE 437. Poly(β-caprolactone) as a polymeric material for orthopaedic implants in the presence of *Staphylococcus aureus*. **M. Steffen**, R.M. Van Horn

PMSE 438. Extrusion based 3D printing of rocket propellant grains. **J. Strutton**, J. McCollum, S.T. Iacono

PMSE 439. Bridging the performance gap: Relating thermomechanical properties to polymer composition in polyester-urethane thermoset coatings. **J. Tilly**, D. Inglefield, S. Khan, R.J. Spontak

PMSE 440. Characterizing nanostructural degradation from accelerated aging in polymer membranes. **M. Toomey**, K. Huang, L. Kearney, A. Shah, J.A. Howarter

PMSE 441. Solventless synthesis of fully bio-based benzoxazine polymers from phloretic acid, polyethylene glycol and furfurylamine. **A. Trejo Machin**, P. Verge, L. Puchot, R. Quintana

PMSE 442. Statistical mechanics of theta-shaped and ring-shaped polymer chains. **E. Uehara**, T. Deguchi

PMSE 443. Tailoring the mechanics and degradation of polyester fibers through manipulating structure and morphology. **K. Van de Voorde**, A.M. Jordan, V. Viswanath, J.K. Pokorski, L. Korley

PMSE 444. Effect of phase separation on water barrier properties in epoxy/amine thermosetting polymers. **J. Vergara**, I. Donahue, J.J. La Scala, J.M. Sadler, S.K. Yadav, G. Palmese

PMSE 445. Tailor-made core-shell particles and shear-induced Aasembly for the preparation of isoporous nanostructures. **S. Vowinkel**, M. Gallei

PMSE 446. Preparation and properties of hydroxyl rich microporous polymer. H. Gong, L. Zhao, **J. Wang**

PMSE 447. Fabrication and characterization of poly (2-hydroxyethyl methacrylate)-based hydrogel membranes. **M. Wang**, O. Heinz, J. Martinez, Y. Ding

PMSE 448. Graphene oxide modified poly(piperazine-amide)/PMIA composite nanofiltration membrane with improved flux and antifouling properties. **T. Wang**, X. He, J. Chen, J. Li

PMSE 449. Intramolecular cross-linking of poly(styrene-*b*-lactide)s for decreasing domain sizes in microphase-separated structures. **K. Watanabe**, S. Katsuhara, T. Isono, T. Yamamoto, K. Tajima, T. Satoh

PMSE 450. Elucidating the effects of extended branch architecture in linear-dendritic block copolymers (LDBCs). **J.S. Williams**, I. Chandrasiri, D. Abebe, D.L. Watkins

PMSE 451. Integrating prior knowledge and machine learning for efficient design of high thermal conductivity polymers. **S. Wu**, Y. Kondo, I. Kuwajima, G. Lambard, K. Hongo, J. Morikawa, Y. Xu, R. Yoshida

PMSE 452. Comparison of the chain structures between high-speed extrusion coating polyethylene resins by preparative temperature rising elution fractionation and cross-fractionation. **Y. Xue**, S. Bo, X. Ji

PMSE 453. Single-digit nanometer polysiloxane-based block copolymers: Design, synthesis, and perpendicular orientation control. **S. Yamazaki**, R. Odashima, T. Seshimo, Y. Nabae, T. Hayakawa

PMSE 454. Harvesting irregular mechanical energy by triboelectric nanogenerator based on cost-effective thermoplastic polymer nanofiber. **S. Yan**, R. Xiao

PMSE 455. Synthesis of novel polyimides containing pyridine units with good comprehensive properties via copolymerization. **M. Yang**, C. Zhang, Y. Dong, L. Tong

PMSE 456. pH-dependent release of anticancer drug doxorubicin from biocompatible thermoresponsive polymersomes. **Y. Yang**, V.A. Kozlovskaya, F. Liu, K. Ingle, A. Ahmad, G. Halade, E.P. Kharlampieva

PMSE 457. Synthesis and self-assembly of poly(styrene-*block*-methyl methacrylate) end-capped with oligosaccharide. **K. Yoshida**, S. Tanaka, K. Miyagi, T. Isono, T. Yamamoto, R. Borsali, K. Tajima, T. Satoh

PMSE 458. Effect of fluoroalcohol on atom transfer radical polymerization of styrene bearing electron-donating group. **H. Yoshioka**, K. Yamaguchi, M. Kobayashi

PMSE 459. Preparation of poly(AM-AMPS-NVP)/SiO_2 nanocomposite microspheres with temperature and salinity resistance in deep drilling fluid. **Y. Zhao**, Y. Ke, Y. Pei

Section A
Ernest N. Morial Convention Center
Hall D

Joint PMSE-POLY Poster Session

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

Cosponsored by POLY
M. Becker, *Organizer*

6:00–8:00

PMSE 460. Chemical recycling of polystyrene wastes: An inherently green fire-retardant poly(vinyl benzoxazine) from expanded polystyrene waste. C. Wang, Y. Liu, Z. Tu, **L. Cheng-Mei**

Integrating Polymer Science in the Curriculum
Sponsored by POLY, Cosponsored by CHED and PMSE

International Symposium on Biorelated Polymers: Innovations in Biomedical Polymers
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Nonlinear Dynamical Approaches to the Synthesis of Polymeric Materials
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Polymer Colloids: Synthesis, Analysis, Modeling & Applications
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Polymer Networks: Soft Gels to Stiff Networks
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Undergraduate Research in Polymer Science
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WEDNESDAY MORNING

Section A
New Orleans Marriott Canal Street
La Galerie 6

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Processing-Structure-Property Relationships

Cosponsored by WCC
Financially supported by DuPont
Z. Bao, Y. Diao, G. Wang, *Organizers, Presiding*

8:30 PMSE 461. Design strategy for efficient thermally activated delayed fluorescence (TADF) organic emitters: From twisted to planar structures. **J.E. Bredas**

9:00 PMSE 462. Quantitation and optimization of process-structure-property relationships in polymer organic electronics. N. Persson, M. McBride, E. Reichmanis, **M. Grover**

9:30 PMSE 463. Directing molecular assembly inspired by living systems. **Y. Diao**

10:00 Intermission.

10:15 PMSE 464. Sulfur in materials science: From polymers to a fully rechargeable lithium battery. **F. Wudl**

10:45 PMSE 465. Plastic semiconductors: How we can exploit blending to manipulate functions? **N. Stingelin**

11:15 PMSE 466. Shear printed conjugated polymers: From microstructure design to integrated soft electronics. **G. Wang**, A. Facchetti, T.J. Marks

Section B
New Orleans Marriott Canal Street
La Galerie 4

Symposium for Pan-American Science

Financially supported by ACS Brazil Chapter
B.D. Olsen, *Organizer*
C. Ornelas, *Organizer, Presiding*

9:00 PMSE 467. Visualization of sodium deoxycholate supramolecular gels with fluorescence probes. S.G. Talluri, **C. Bohne**

9:30 PMSE 468. Surface modifying cellulose nanofibrils towards multifunctional aerogels. **C.G. Otoni**, J.S. Figueiredo, M. Mariano, J.d. Bernardes, W. Loh

9:50 PMSE 469. Ion-selective and high capacity electrodes for membrane capacitive deionization. A. Jain, J. Kim, K. Zuo, Q. Li, **R. Verduzco**

10:20 PMSE 470. Recent advancements in polyelectrolytes. **L.M. Campos**

10:50 Concluding Remarks.

Section C
New Orleans Marriott Canal Street
Studio 3

‡*Cooperative Cosponsorship*

Polymers with Complex Architecture: From Synthesis to Self-Assembly

Financially supported by NSF, BASF, ExxonMobil, LG MMA, and Wyatt Technology, Department of Chemistry & Biochemistry at Florida State University
J.G. Kennemur, M. Seo, G. Stein, *Organizers*
C.Y. Ryu, *Organizer, Presiding*

8:30 PMSE 471. Synthesis and characterization of new polyolefin comb blocks comprised of a poly(ethylene-co-acrylic acid) scaffold and polypropylene arms: Exploration of the impact of number, length, and crystallinity of the grafted arms on melt and solid state properties. **P. Brant**, C.R. Lopez-Barron

9:00 PMSE 472. Towards next generation polyolefin standards: Controlled synthesis of short-chain branched polyethylene *via* ring-opening metathesis polymerization. **W. Farrell**, S.V. Orski, K. Beers

9:20 PMSE 473. Crystallization of precision polyethylenes with acetal groups. **X. Zhang**, S. Cameron, P. Ortmann, S. Mecking, R.G. Alamo

9:40 PMSE 474. Photo-controlled growth of crosslinked nano-networks. **M.W. Lampley**, E. Harth

10:00 Intermission.

10:15 PMSE 475. LGMMA R&D strategy and product development roadmap. **Y. Lee**, M. Seo

10:35 PMSE 476. Synthesis of epoxy networks and interphases with controlled topology. **J. Gao**, G. Palmese

10:55 PMSE 477. Supramolecular design principles for the synthesis of 2D covalent organic frameworks. **R. Smaldone**, G. Occhialini, C. Thompson, S.O. Nielsen

11:15 PMSE 478. Synthesis and characterization of "Janus-type" linear-dendritic block copolymers (LDBCs) for therapeutic applications. **I. Chandrasiri**, D. Abebe, J.S. Williams, S. Gupta, G. Schneider, D.L. Watkins

11:35 PMSE 479. Temperature-triggered loading and release of hydrophobic model drugs in free-standing multilayer films for nano-adhesive patches. **R. Saikaew**, S.T. Dubas

Section D
New Orleans Marriott Canal Street
La Galerie 5

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

P. Froimowicz, I. Hamerton, H. Ishida, *Organizers*
R.C. Advincula, C. Jubsilp, *Presiding*

8:00 PMSE 480. Benzoxazine dimer and polybenzoxazine for as-desiged functions and phenomena. **S. Chirachanchai**

8:40 PMSE 481. Withdrawn

9:10 PMSE 482. Design of high performance thermosets asymmetric benzoxazines from lignin derivatives and vegetable oils. L. Puchot, C. Vancaeyzeele, F. Vidal, P. Verge, **Y. Habibi**

9:30 PMSE 483. Design and preparation of fully bio-based polybenzoxazine from amino acid. W. Li, X. Zhang, W. Shi, **X. Jia**

9:50 PMSE 484. High performance ceramic-based benzoxazine micro and nanocomposites. **M. Derradji**, L. Wenbin

10:10 Intermission.

10:20 PMSE 485. Poly(vinyl benzoxazine): A novel kind of green intrinsic fire-retardant thermoplastics with high molecular weight. Y. Cao, H. Ma, Y. Liu, Z. Tu, **L. Cheng-Mei**

10:40 PMSE 486. Alternative approach in preparation of the maleimidobenzoxazines. **Z. Stirn**, A. Ručigaj, M. Krajnc

11:00 PMSE 487. Ultrathin coating containing high nanofiller: Superior flame retardancy performance of intercalation/exfoliation to non-intercalation of benzoxazine surfactant modified clay with natural polymer. **F. Shan**

11:20 PMSE 488. Mussel-inspired benzoxazines for thermoset resins and adhesives. **C.J. Higginson**, P.B. Messersmith

11:40 PMSE 489. Withdrawn

Section E

New Orleans Marriott Canal Street
Studio 5

General Papers: New Concepts in Polymeric Materials
Cosponsored by WCC
M. Becker, *Organizer*
C. O'Brien, L. Zhai, *Presiding*

8:30 PMSE 490. Role of isosorbide comonomer on interfacial tension with subsequent mophologies & mechanical properties of biobased poly(L-lactide)/poly(ethylene-co-isosorbide terephtalate) blends. **A. Bouzouita**, C. Samuel, T. parpaite, M. Lacrampe, M. Collinet, S. Bourbigot, G. Fontaine, S. Marcille, H. Amedro, J. Soulestin

8:55 PMSE 491. Study on poly(3-dodecylthiophene) behavior during heating and stretching by *in-situ* small and wide-angle X-ray scattering. **H. Chen**, G. Liu, D. Wang

9:45 PMSE 492. Mutifunctional polyelectrolyte fibers with metal ions. **L. Zhai**, X. Lu, A. Malhotra

10:10 Intermission.

10:25 PMSE 493. Conductive polyamide–graphene composite fabric via interface engineering. **C. Sutanto**, E. Barjasteh, D. Nepal

10:50 PMSE 494. Fabricating millifluidic devices for SAXS/WAXS using 3D printing; a quick and inexpensive method to exploit many geometries. **C. O'Brien**, N.J. Terrill, O. Mykhaylyk, A. Ryan

11:15 PMSE 495. Galloyl groups-regulated fibrinogen conformation: Understanding antiplatelet adhesion on tannic acid coating. **L. Yang**, L. Han, L. Jia

11:40 PMSE 496. Mass and charge transport in organic radical polymers (Rising Star award address). **J.L. Lutkenhaus**

Section F
New Orleans Marriott Canal Street
Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

8:30 PMSE 497. Preparation of three-dimensional polymers with movable cross-linking points via pseudopolyrotaxane. **M. Kubo**, M. Okuro, T. Kawashima, T. Uno, T. Itoh

9:00 PMSE 498. Poly[*n*]catenanes: The synthesis of molecular interlocked chains. **Q. Wu**, X. Lang, P.M. Rauscher, R.J. Wojtecki, J.J. De Pablo, M. Hore, S.J. Rowan

9:20 PMSE 499. Nano knitting and "knotting"–single-chain nanoparticles. **E.B. Berda**, E.R. Bright, R. Chen, J. Cole

9:40 PMSE 500. Dithiacrown ethers as the cyclic component of polyrotaxanes and as the ligand of transition metal complexes. **K. Osakada**

10:00 Intermission.

10:10 PMSE 501. Cyclic monomers for supramolecular polymerization and enforced entanglements. **H.W. Gibson**, T. Price, H. Wessels, C. Slebodnick, A.L. Rheingold, N. Pothanagandhi

10:40 PMSE 502. Being knotty with supramolecular polymers. **R.C. Advincula**

11:10 PMSE 503. On-surface synthesis of polymers and macrocycles. **J. Gottfried**, Q. Fan, J. Zhu, C. Krug, K. Greulich

Section G
New Orleans Marriott Canal Street
Studio 9

Additive Manufacturing of Structures & Functional Devices: Materials, Methods, Models & Testing

Process Improvement & Understanding

D. Berrigan, J. Lewis, *Organizers*
C.R. Snyder, *Organizer, Presiding*

8:30 PMSE 504. Process engineering for digital manufacturing. **C.F. Fox Converse**

9:00 PMSE 505. Molecular weight dependence of polycarbonate weld formation in material extrusion additive manufacturing. **J. Seppala**

9:20 PMSE 506. Enhancing thermomechanical properties of PMMA parts fabricated via fused deposition modeling by incorporation of polymer-grafted nanoparticles. **D.P. Street**, J.A. Bergman, J.M. Messman, M. Kilbey

9:40 PMSE 507. Quantifying reversibility in 3D printed networks using hetero-Diels-Alder linkages. **W. Korf**, Y.C. Simon

10:00 Intermission.

10:15 PMSE 508. Effects of material extrusion parameters on the properties of crystallizing polycaprolactones for additive manufacturing. **A. Kotula**, K. Migler

10:45 PMSE 509. Improving anisotropic properties of objects printed via stereolithography. **B. Green**, R. McLeod, A. Guymon

11:05 PMSE 510. Direct ink writing of ceramic and cementitious materials. **J.P. Youngblood**, R. Trice, L. Rueschhoff, W. Costakis, A. Diaz, P. Zavattieri, J. Olek, M. Moini

11:25 PMSE 511. Enhanced green part strength in binder jet additive manufacturing. D.B. Gilmer, E. Hong, A. Kisliuk, S. Cheng, A. Elliott, **T. Saito**

International Symposium on Biorelated Polymers: Renewable Materials

Functionalization & Modification of Renewable Feedstocks

Sponsored by POLY, Cosponsored by PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

Biobased Gels & Porous Materials

Functionalised Nanocellulose Gels

Sponsored by CELL, Cosponsored by COLL and PMSE

Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

WEDNESDAY AFTERNOON

Section A
New Orleans Marriott Canal Street
La Galerie 6

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Frontiers in Chemistry of Materials

Cosponsored by WCC
Financially supported by DuPont
Z. Bao, Y. Diao, G. Wang, *Organizers, Presiding*

1:30 PMSE 512. Hybridizing organic and inorganic materials for unconventional electronics. **T.J. Marks**

2:00 PMSE 513. Materials engineering for addressing global inflections in

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electronics, display, energy, additive manufacturing and other emerging markets. **O. Nalamasu**

2:30 PMSE 514. Self-assembly of block copolymer nanopatterns on surfaces. **J.M. Buriak**, C. Jin, E.J. Luber, B. Olsen

3:00 Intermission.

3:15 PMSE 515. Flexible and stretchable electronics. **Z. Bao**

3:45 PMSE 516. Determining the orientation of molecular dipoles on random 2D nanoplasmonic structures. **T.A. Purcell**, T. Seideman

4:15 PMSE 517. Award Address (ACS Award in the Chemistry of Materials Sponsored by DuPont). From silicon to plastic: Materials design and process considerations. **E. Reichmanis**

Section B
New Orleans Marriott Canal Street
La Galerie 4

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
K. Golovin, F. Yang, *Presiding*

1:30 PMSE 518. Functional microgel-based microfibres. **A. Pich**

1:55 PMSE 519. Improvement of the mechanical performance of pectin/GO composite films after non-covalent functionalization of graphene oxide. **A.M. Pandele**

2:20 PMSE 520. Development of a predictive framework for the design and fabrication of icephobic polymers. **K. Golovin**

2:45 PMSE 521. Semi-crystalline block copolymers as fat crystal habit modifiers. **J. Jennings**, M. Butler, O. Mykhaylyk, A. Ryan

3:10 Intermission.

3:25 PMSE 522. Facile loading of gold nanoparticles and gadolinium within alginate nanogels for enhanced dual mode tumor MR/CT imaging. **W. Sun**, J. Zhang, C. Peng, X. Shi

3:50 PMSE 523. Synthesis and characterization of cardanol-based epoxy/amine systems and analysis of secondary epoxies. **E. Kinaci**, E. Can, J. La Scala, G. Palmese

4:15 PMSE 524. Super bulk and interfacial toughness of fully physically-crosslinked double-network hydrogels. **Y. Zhang**, B. Ren, H. Chen, F. Yang, Y. LIU, J. Zheng

4:40 PMSE 525. Novel design of multi-mechanoresponsive and mechanically strong hydrogels. **F. Yang**, Y. Zhang, H. Chen, B. Ren, Y. Liu, J. Zheng

Section C
New Orleans Marriott Canal Street
Studio 3

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
X. Guo, L. Williams, *Presiding*

1:30 PMSE 526. Templated synthesis of polymer microparticles with complex anisotropic shapes and internal morphologies. **X. Guo**, Y. Kim, Y. Yang, K.d. Santiago Gonzalez, S. Spagnolie, N.L. Abbott, D.M. Lynn

1:55 PMSE 527. Towards a long-chain perfluoroalkyl replacement: wettability of polymer films modified with perfluoropolyethers-based triblock copolymers. **L. Wei**, T. Demir, I.A. Luzinov, P. Brown

2:20 PMSE 528. Withdrawn

2:45 Intermission.

3:00 PMSE 529. Formation of polybutene-1 hexagonal crystals directly from melt within confined microdomains. **Z. Wang**, D. Wang

3:25 PMSE 530. Withdrawn

3:50 PMSE 531. Novel nanoparticle network design and investigation of their structure-property relationships. **L. Williams**, E. Harth

Section D
New Orleans Marriott Canal Street
La Galerie 5

Third International Symposium on Polybenzoxazines: Towards Diamond Jubilee of Benzoxazine Chemistry

P. Froimowicz, I. Hamerton, H. Ishida, *Organizers*
D. Lomonaco, Q. Ran, *Presiding*

1:30 PMSE 532. Fabrication and properties of polybenzoxazine-based functional surface. **Z. Xin**

2:05 PMSE 533. Multifunctional and lightweight composites based on high performance benzoxazine matrices. **L. Bonnaud**, L. Dumas, O. Murariu, M. Poortman, M. Olivier, P. Dubois

2:35 PMSE 534. Preparation and Characterization of β-ZrP / Polybenzoxazine Nanocomposites. **Y. Li**

3:05 PMSE 535. Unconventional applications of benzoxazine chemistry for advanced materials. **B. Kiskan**, M. Arslan, Y. Yagci

3:35 Intermission.

3:50 PMSE 536. Corrosion resistance of diamine-based polybenzoxazine coating on mild steel. X. Lu, R. Zhang, C. Zhou, **Z. Xin**

4:10 PMSE 537. Effects of reaction solvents on the chemical structure and high frequency dielectric property of main chain type benzoxazine copolymers. **M. Zeng**, J. Chen, Q. Xu, D. Yin, Z. Feng, T. Pang, S. Zeng, Y. Huang, Y. Gu

4:30 PMSE 538. Polybenzoxazine graft copolymers from miscible blends of polymers with thermally labile groups. **D.A. Rider**

4:50 PMSE 539. Thermal and mechanical properties of novel maleimidobenzoxazines prepared via phenolic diversity of reactants. **A. Ručigaj**, Z. Stirn, M. Krajnc

5:10 PMSE 540. Structure-flammability correlations of benzoxazines. **J. George**, F. Shan, H. Ishida

Section E
New Orleans Marriott Canal Street
Studio 5

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
A. Mueller, L. Rueschhoff, *Presiding*

1:30 PMSE 541. Patterning of preceramic polymers via macromolecular self-assembly. **L. Rueschhoff**, L. Baldwin, D. Berrigan, H. Koerner, T. Pruyn, M. Dickerson

1:55 PMSE 542. Diels-Alder crosslinked hydrogels enable 3D cell encapsulation with increased reactivity. **L.J. Smith**, R.Y. Tam, S. Taimoory, A.E. Baker, J.F. Trant, M.S. Shoichet

2:20 PMSE 543. Poly(ethylene glycol) brushes for efficient siRNA delivery. **D. Wang**, K. Zhang

2:45 PMSE 544. Fluorinated polyeletrolytes as single ion conductors for Li batteries. **W. Zhang**, S. Feng, M. Huang, Y. Shao-Horn, J.A. Johnson

3:10 Intermission.

3:25 PMSE 545. Long-chain branching on polyamide 6 through reaction extrusion for melt foaming. M. Xu, **T. Liu**

3:50 PMSE 546. Perfluorinated block-copolymers for dry proton exchange membranes. A. Argall, C. Hager, M.J. Quast, **A. Mueller**

4:15 PMSE 547. pH-Responsive polysaccharide-modified liposomes for antigen delivery and induction of immune responses. **E. Yuba**, A. Yamaguchi, S. Uesugi, A. Harada, K. Kono

Section F
New Orleans Marriott Canal Street
Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

1:30 PMSE 548. Topologially complex hydrogels. **R.M. Waymouth**

2:00 PMSE 549. It's all about topology: The evolution of polymer brushes and their performance. G. Morgese, M. Divandari, **E. Benetti**

2:30 PMSE 550. Synthesis of cyclic polymers and control of their properties. **T. Yamamoto**

3:00 Intermission.

3:10 PMSE 551. Rings, stars, and dense brushes grown from flat substrates and spherical nanoparticles: How polymer topology perturbs glass transition temperature and fragility in bulk and confined states from linear polymer behavior. **J.M. Torkelson**, L. Zhang, T. Lan, S. Askar, L. Li, R. Elupula, S.M. Grayson

3:40 PMSE 552. Crystallization of poly(β-caprolactone) under topological and thin film confinement. **J. Albert**, G. Kelly, F.M. Haque, S.M. Grayson

4:10 PMSE 553. Influence of chain topology on polymer crystallization and glass temperature: Rings vs. linear chains. **G. Floudas**, A. Pipertzis, M. Monteiro

Section G
New Orleans Marriott Canal Street
Studio 9

Additive Manufacturing of Structures & Functional Devices: Materials, Methods, Models & Testing

Soft Robotics, Electronics & Actuation

D. Berrigan, J. Lewis, C.R. Snyder, *Organizers*
J. Seppala, *Presiding*

1:30 PMSE 554. Evolution of soft robotics. **R. Shepherd**

2:00 PMSE 555. 3D printable, self-healing, viscoelastic conducting polymer for wearable electronics applications. **Y. Wang**

2:20 PMSE 556. Multi-material additive manufacturing with solution mask liquid lithography (SMaLL). **N. Dolinski**, Z.A. Page, B. Callaway, F. Eisenreich, R. Garcia, R. Chavez, D. Bothman, S. Hecht PhD, F. Zok, C.J. Hawker

2:40 PMSE 557. Hierarchical co-assembly enhanced direct ink writing. **C. Ke**

3:00 Intermission.

3:15 PMSE 558. Multimaterial 3D printing for shape changing devices and 4D printing. Z. Ding, C. Yuan, M. Dunn, **H. Qi**

3:45 PMSE 559. 4D printing of TPU nanocomposite actuators. **R.C. Advincula**

4:05 PMSE 560. Additive manufacturing of hydrogel composites by direct-write 3D printing. **A. Nelson**

4:25 PMSE 561. Self-organized interpenetrating polymer network in semiconducting films for stretchable electronics. **G. Zhang**, E. Reichmanis

International Symposium on Biorelated Polymers: Renewable Materials

Synthesis of Renewable Materials

Sponsored by POLY, Cosponsored by PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage
Sponsored by ENFL, Cosponsored by CATL, INOR and PMSE

Biobased Gels & Porous Materials

Cellulose & Non-Cellulose Gels: Synthesis, Properties, Applications

Sponsored by CELL, Cosponsored by COLL and PMSE

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Polymer Colloids: Synthesis, Analysis, Modeling & Applications
Sponsored by POLY, Cosponsored by ANYL, COLL, COMP, I&EC and PMSE

WEDNESDAY EVENING

POLY/PMSE Plenary & Awards Event
Sponsored by POLY, Cosponsored by PMSE‡

THURSDAY MORNING

Section A
New Orleans Marriott Canal Street Beauregard

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
M. Cui, S. Manna, I. Zvonkina, *Presiding*

8:30 PMSE 562. Design of polymeric NLRP3-TLR agonist conjugates as vaccine adjuvants. **S. Manna**, W.J. Howitz, N.J. Oldenhuis, A. Eldredge, M. Lodeon, Z. Guan, A.P. Esser-Kahn

8:55 PMSE 563. Nanoscale ion-gel films as gate insulator material retaining high capacitance at megahertz switching frequency enabled by initiated chemical vapor deposition (iCVD). **M. Wang**, A. Liu, S. Schroeder, J. Zhao, K. Gleason

9:20 PMSE 564. Chain extension of polyamide 6 using multifunctional chain extenders and reactive extrusion for melt foaming. M. Xu, **T. Liu**, C. Park

9:45 PMSE 565. 'Nano-ruler' for chain dimension and molecular conformation in ultrathin polymer films based on surface contact angle. **I. Zvonkina**, A. Karim

10:10 Intermission.

10:25 PMSE 566. Highly stretchable sustainable electronic skin sensor with real-time self-healing. **M. Cui**, N. Nguyen, K. Meek, A.K. Naskar

10:50 PMSE 567. Carbon nanofiber production from electrospinning of liquid residue derived from supercritical CO2-ethanol extraction of Powder-River-Basin coal. **M. Tang**, F. Liu, X. He, K. Sun, M. Fan

11:15 PMSE 568. Sugar poly(orthoesters) to construct highly pH-responsive nanoscopic assemblies. **W. Du**, S. Maiti

Section B
Astor Crowne Plaza New Orleans Burgundy

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
M. Krecker, H. Verma, *Presiding*

8:30 PMSE 569. Assembly of grafted polymers on modified graphene oxide. **M. Krecker**, A.M. Grant, M. Savchak, N. Borodinov, I.A. Luzinov, V.V. Tsukruk

8:55 PMSE 570. Low resistant and high water flux membranes improve the energy efficiency of membrane capacitive deionization. **V. Palakkal**, C. Arges

9:20 PMSE 571. Ordered bicontinuous nanostructures in a rod-coil block copolymer. **Z. Shen**

9:45 Intermission.

10:00 PMSE 572. Supported iron and tungsten nanoparticles incorporated polymer composites with uniform and static dispersion. **T. Hussain**, F. RIAZ, A. Mujahid, K. Shehzad

10:25 PMSE 573. Rolling and sliding friction characterization of polystyrene microspheres (PS) using force spectroscopy and lateral force microscopy. **H. Verma**, W.G. Matthews

10:50 PMSE 574. Prepreparation and flame retardant performance characterization of a novel self-intumescent spirocyclic flame retardant. **D. Wang**, S. Li, J. Liu

Section C
New Orleans Marriott Canal Street Studio 3

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
L. Ju, M. Korey, *Presiding*

8:30 PMSE 575. Phosphonated poly(ethylene terephthalate) ionomer: Effects of divalent anion on thermal and rheological properties of polyester ionomer. **L. Ju**, J. Pretelt, J.M. Dennis, K.A. Valentine, D.G. Baird, T.E. Long, R.B. Moore

8:55 PMSE 576. Substrate independent approach to dense cleavable polymer brushes from a coating by nitroxide mediated polymerization. **W. Wei**, B. Ayyakkalai, P. Gopalan

9:20 PMSE 577. Oligoanilines grafted membranes for water ultrafiltration. **C. Lin**, S. Aguilar, X. Huang, J. Tulyagankhodjaev, R.B. Kaner

9:45 PMSE 578. Biodegradable and stretchable multi-block semiconducting copolymers. F. Sugiyama, **A. Kleinschmidt**, M. Alkhandra, J. Wan, A. Chiang, D. Rodriquez, S. Root, S. Savagatrup, D.J. Lipomi

10:10 Intermission.

10:25 PMSE 579. Fluoranthene containing porous organic polymers for fluorescense sensing. **C. Thompson**, G. Occhialini, R.A. Smaldone

10:50 PMSE 580. Acetylated tannic acid as a more sustainable alternative to brominated flame retardants in epoxy. **M. Korey**, N. Burgos, J.P. Youngblood, J.A. Howarter

11:15 PMSE 581. Vertically oriented block copolymer thin film by dynamic thermal field directd self-assembly. M. Basutkar, D. Raghavan, A. Elzatahry, **A. Karim**

11:40 PMSE 582. Tip-enhanced optical techniques for chemical nanomapping. **S.I. Leesment**, V.V. Polyakov, A.V. Shelaev

Section D
Astor Crowne Plaza New Orleans Bourbon

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
N.R. Mammoottil, S.R. Nowak, *Presiding*

8:30 PMSE 583. Substituent effects on the pH sensitivity of acetals and ketals and their correlation with encapsulation stability in polymeric nanogels. **B. Liu**, S. Thayumanavan

8:55 PMSE 584. Fabrication and characterization of ultra-thin films of thermoresponsive, nanostructured sugar-polyolefin amphiphilic conjugates. **S.R. Nowak**, K.K. Lachmayr, L.R. Sita

9:20 PMSE 585. Integrating metal sulfide nanoparticles with porous PMMA membranes for desulfurization applications. **A. Mujahid**, A. Maryam, T. Hussain, S. Bajwa

9:45 PMSE 586. Dependence of sidechain structure on the morphology and properties of perfluorinated ionomers. **C.M. Orsino**, R.B. Moore

10:10 Intermission.

10:25 PMSE 587. Controlled release of camptothecin from functional polyphosphonamidate nanoparticles exhibiting acid-triggered degradation. **H. Wang**, L. Su, R. Li, M. Dong, K.L. Wooley

10:50 PMSE 588. Fracture behavior of thermoplastic films in outdoor and accelerated laboratory exposure. **A. Fairbrother**, H. Hsueh, J. Kim, D. Goodwin, L. Perry, S.J. Watson, C.C. White, X. Gu, L. Sung

11:15 PMSE 589. Scanning probe nanomechanical characterization of PS-LDPE copolymer using cantilever probes with varying stiffness. **W. Shi**, G. Pascual, A. Zandiatashbar, B. Kim, K. Lee

11:40 PMSE 590. Unique surface re-organization and vapor sensitivity of PNOC. **N.R. Mammoottil**, J.F. Reuther, R. Campos, B.M. Novak

Section E
New Orleans Marriott Canal Street Studio 2

General Papers: New Concepts in Polymeric Materials

M. Becker, *Organizer*
L.A. Baldwin, X. Chen, *Presiding*

8:30 PMSE 591. Unique crystallization behavior of isotactic polypropylene in the presence of L-isoleucine and Its inhibition and promotion mechanism of nucleation. **S. Zhao**, X. Peng, Z. Xin

8:55 PMSE 592. Self-assembled graphene composites as porous electrodes for energy storage. **D. Varghese**, D.H. Adamson, E. Gentile, C. Schilling

9:20 PMSE 593. Soluble polymers with intrinsic porosity for flue gas purification and natural gas upgrading. **X. Wang**, **Z. Lai**

9:45 PMSE 594. Concentration fluctuation during nucleation in a phase separating broad ethylene copolymer leads to partial dissolution of melt memory. **X. Chen**, C.R. Lopez-Barron, Y. Zeng, R.G. Alamo

10:10 Intermission.

10:25 PMSE 595. Effect of partial saturation on thermodynamic interactions in polydiene/polyolefin blends. **J. Qiu**, C.R. Lopez-Barron, M.L. Robertson, R. Krishnamoorti

10:50 PMSE 596. Hyperbranched polycarbosilanes for modular synthesis of ceramics. **L.A. Baldwin**, L. Rueschhoff, H. Koerner, M.J. Dalton, M. Dickerson

11:15 PMSE 597. Oxime hyaluronan hydrogels as a model for breast cancer. **A.E. Baker**, R.Y. Tam, A. Ganesh, L. Bahlmann, N. Mitrousis, J. Liu, G. Bader, M.S. Shoichet

11:40 PMSE 598. Molecular gel composites: From solution to solid-state reversibility. **S. Alexander**, L. Korley

Section F
New Orleans Marriott Canal Street Studio 8

Cyclic & Topologically Complex Polymers
Cosponsored by POLY
Financially supported by MilliporeSigma; Tosoh Biosciences LLC; Zeon Corporation; Toyo Styrene Co., Ltd.; Elsevier
S.M. Grayson, Y. Tezuka, *Organizers, Presiding*

8:30 PMSE 599. Playing with the rings. **N. Hadjichristidis**, G. Polymeropoulos, Y. Jiang, N. Alkayal, Z. Zhang, D. Wang, P. Bilalis

9:00 PMSE 600. Synthesis and properties of stimuli-responsive linear and cyclic graft copolymers bearing multifunctional Y junctions. **Y. Zhao**, W. Dai, J. Zhang, X. Zhao, W. Wu

9:30 PMSE 601. Multiply-controlled cyclic polymers prepared by controlled/living and stereospecific polymerizations. **K. Satoh**, M. Kamigaito

10:00 Intermission.

10:10 PMSE 602. Universal scaling model for linear and cyclic block copolymer domain spacing from dissipative particle dynamic (DPD) simulation. **A. Goodson**, J.N. Albert, H. Ashbaugh

10:30 PMSE 603. Versatile nanomicelle carrier platform self-assembled by brush cyclic and tadpole copolymer amphiphiles. **B.J. Ree**, Y. Satoh, K. Jin, T. Isono, W. Kim, T. Kakuchi, T. Satoh, M. Ree

10:50 PMSE 604. Promoting cyclic morphologies in an acrylate-based metallo-supramolecular network. **A.M. Savage**, R.H. Lambeth, F.L. Beyer

11:10 PMSE 605. Solution self-assembly of block copolymers of branched architectures. **K. Kim**

11:30 Concluding Remarks.

Section G
New Orleans Marriott Canal Street Studio 9

Additive Manufacturing of Structures & Functional Devices: Materials, Methods, Models & Testing

Novel Materials & Materials Improvements

D. Berrigan, J. Lewis, C.R. Snyder,

‡*Cooperative Cosponsorship*

Organizers
A. Kotula, *Presiding*

8:30 PMSE 606. Effect of chain alignment on thermal welding in fused filament fabrication. M. Galvani, T. O'Connor, T. Ge, **M.O. Robbins**

9:00 PMSE 607. Balancing surface energy and reactivity in binary polymer blends: Development of 3D-printed energetic composites. **J. McCollum**, J. Bencomo, S.T. Iacono

9:20 PMSE 608. Thiol-enhanced photocuring of high-performance cyanate ester resins for additive manufacturing. **S. Hosseini**, B. Lund, W. Voit

9:40 PMSE 609. Preparation and properties of fire prevention insulation expanded vermiculite composites. **D. Wang**, J. Liu

10:00 Intermission.

10:15 PMSE 610. Shelf-stable photo-curable resins for mechanically robust additively manufactured parts. **W. Voit**, J. Huffstetler, B. Lund

10:35 PMSE 611. Modifying the rheological properties of ABS resins for 3D printing applications. **Y. Bai**, J.H. Wang, C. Shen

10:55 PMSE 612. Influence of nanoclay morphology on the printability of fiber-reinforced composite inks. **K. Johnson**, A. Abbott, J. Baur, H. Koerner

11:15 PMSE 613. 3D printing with polymeric nanogel particles. **P.K. Shah**, J.W. Stansbury, R. McLeod, A.C. Uzcategui, M. Eulau

11:35 PMSE 614. Polymeric nanophotonic devices for abrupt control of optical beams in three dimensions. **S.M. Kuebler**, R. Sharma, J.L. Digaum, N. Kosan, N. Martinez, C.L. Valle, R.C. Rumpf

International Symposium on Biorelated Polymers: Renewable Materials

Renewable Polyesters

Sponsored by POLY, Cosponsored by PMSE

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

Biobased Gels & Porous Materials

Biomedical Applications of Polysaccharide Gels & Aerogels

Sponsored by CELL, Cosponsored by COLL and PMSE

THURSDAY AFTERNOON

International Symposium on Biorelated Polymers: Renewable Materials

Properties & Applications of Renewable Materials

Sponsored by POLY, Cosponsored by PMSE

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

Biobased Gels & Porous Materials

Polysaccharide Foams, Cryogels & Aerogels

Sponsored by CELL, Cosponsored by COLL and PMSE

PROF

Division of Professional Relations

R. Libby, *Program Chair*

SUNDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 22

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC
M. Morris, *Organizer*
T. Iannuzzi, *Presiding*

9:00 Introductory Remarks.

9:05 PROF 1. Rhizosphere effects on lamotrigine accumulation by wheat plants. **E.L. Miller**, S.L. Nason, R.M. Hoehn, K.G. Karthikeyan, J.A. Pedersen

9:25 PROF 2. Examination of the specific binding of cytochrome c on MPA-coated gold nanoparticles via protein footprinting. **E. Tollefson**, X. Zhang, N. Rozanov, C. Allen, C.J. Murphy, R. Hernandez, E.E. Carlson

9:45 PROF 3. Discovery of selective nanomolar potent Melanocortin-3 Receptor ligands. **S.R. Doering**, K.T. Freeman, G. Debevec, P. Geer, R.G. Santos, M.A. Giulianotti, C. Pinilla, J.R. Appel, R.A. Houghten, C. Haskell-Luevano

10:05 PROF 4. Toward libraries of artificial macrocycles using MCR. **E. Abdelraheem**, M. Rudrakshula, A. Rossettia, G. Liao, C. Neochoritis, M. de Haan, P. Patil, S. Shaabani, A. Doemling

10:25 Intermission.

10:35 PROF 5. Understanding selective binding motifs to design arylethynyl urea anion sensors. **L. Eytel**, D.W. Johnson, M.M. Haley

10:55 Introductory Remarks.

11:00 PROF 6. From strength in diversity to smart nanoscale technologies. **D.K. Smith**

SUNDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 22

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC
M. Morris, *Organizer*
S.R. Doering, *Presiding*

1:30 Introductory Remarks.

1:35 PROF 7. Optimizing $YBa_2Cu_3O_7$ superconducting nanocomposites through nanocrystal surface chemistry. **J. De Roo**, H. Rijckaert, K. De Keukeleere, Z. Hens, J.C. Martins, I. Van Driessche

1:55 PROF 8. Imaging crystal growth from nanometers to microns: *In situ* microscopy across scales for the study of europium oxalate growth. **J.A. Soltis**, M. Conroy, E. Buck, G.J. Lumetta

2:15 PROF 9. Identification of key intermediates in iron C-H functionalization. **T. Iannuzzi**, M.L. Neidig

2:35 PROF 10. Ligand imparts redox active character in earth-abundant metal complexes for multielectron processes. **D.L. Ross**, D. Brazzolotto, A. Borovik

2:55 Intermission.

3:10 PROF 11. Thermodynamics of complex metal oxide dissolution. **J.W. Bennett**, D. Jones, R.J. Hamers, S.E. Mason

3:30 PROF 12. Allegory of the cage: Shedding light on order in silicon clathrates. **L.W. Colaciello**, G.A. Hegde, C.M. Maupin, S. Vyas

3:50 PROF 13. Panel discussion: The LGBTQ+ community in chemistry–opportunities, challenges, and perspectives for graduate students and postdoctoral scholars. **M. Morris**

Chemical Angel Network (CAN): Chemists Investing in Chemistry-Based Companies
Sponsored by BMGT, Cosponsored by PROF and SCHB‡

Starting a Successful Research Program at a PUI
Sponsored by YCC, Cosponsored by PROF

Legal Issues for Chemical Companies in the Food, Energy & Water Industries
Sponsored by SCHB, Cosponsored by CHAL and PROF

SUNDAY EVENING

Entrepreneurs' Poster Session
Sponsored by SCHB, Cosponsored by PROF

MONDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 22

The Bond Between Science & Disability, Forging New Capabilities for Inclusion

L.W. Hoffman, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 PROF 14. Increasing participation of students with disabilities in STEM. K.S. Booksh, **S. Rozovsky**

8:25 PROF 15. Does ACS degree requirements marginalize students with disabilities. **K.S. Booksh**

8:45 PROF 16. Dyslexic advantage. **A.E. Norton**

9:05 Intermission.

9:10 PROF 17. Designing for accessability in a blended learning course. **G.L. Heard**

9:30 PROF 18. Experiencing graduate school in chemistry as a blind student. **A.E. Neybert**, R.W. Schwenz

9:50 PROF 19. Blind scientists: A historical perspective on contributions and innovations. **C.A. Supalo**

10:10 PROF 20. Pairing chemistry with blindness: A journey through graduate school and more. **H. Wedler**

10:30 Intermission.

10:35 PROF 21. Serviced dogs in the chemistry laboratory: Some items to consider. **P.A. Redden**

10:55 PROF 22. Insights from experience in mentoring graduate students. **T.L. Windus**

11:15 PROF 23. Expanding biomedical training to the deaf/hard-of-hearing community. **T.E. Pagano**, A.D. Ross, G. Buckley, S.R. Smith, J. DeCaro, S. Dewhurst

11:35 PROF 24. Hiring people with disabilities: Competitive advantage for the savvy manager. **J.J. Johnston**

11:55 Concluding Remarks.

How to Foster Diversity in the Chemical Sciences

Lessons Learned & Taught Through the Stories of Recipients of the Stanley C. Israel Award

Sponsored by CMA, Cosponsored by PROF and WCC

Science of Sexual Harassment

The Psychology & Sociology of Sexual Harassment

Sponsored by WCC, Cosponsored by PRES, PROF and YCC‡

Excellence in Graduate Polymer Research

Polymerization Techniques

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 22

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC
M. Morris, *Organizer*

3:00–5:00

PROF 25. Interaction of fluorescent teixobactin analogues with bacteria. **M.**

‡*Cooperative Cosponsorship*

Morris, M. Malek, J.S. Nowick

PROF 26. Tungsten nitrido precursors for deposition of WN_xC_y thin films. **M.M. Nolan**, A.J. Touchton, S. Kim, T.J. Anderson, L. McElwee-White

PROF 27. Tannic acid: A sustainable crosslinking agent for high glass transition epoxy materials. **M. Korey**, G. Mendis, J.A. Howarter, J.P. Youngblood

PROF 28. Herbariomics: Expanding possibilities for herbaria-based research pipelines by defining the herbariome. **J. de la Parra**

PROF 29. Functionalized NHCs as ligands for molecular cluster. **E. Doud**

PROF 30. Transamination of 7-keto-8-aminopelargonic acid (KAPA) with amino-donor lysine in *Bacillus subtilis*. **S.A. Souza**, J. Morris, J. Jarrett, H. Ng

PROF 31. Hypoglycemic, hypolipidemic and antioxidant properties of a combination of curcumin from Curcuma Longa, Linn, and partially purified product from Abroma Augusta, Linn, in streptozotocin-induced diabetes. **H.M. Eshrat**

PROF 32. Building a better house: A new approach to Mesoporous silica nanoparticle synthesis. **L. Chlebanowski**, J. Yu, F. Wolschendorf, D.L. Troyer, S.H. Bossmann

PROF 33. $Li_2Mg_2Si_2S_8$ and $Li_2Mg_2Ge_2S_6$: two new quaternary lithium sulfides with potential in infrared nonlinear optics. **C. Barton**, S.S. Stoyko, W. Zhang, S. Halasyamani, J.A. Aitken

PROF 34. Electronic communication in heterotrimetallic systems incorporating the redox-active $M[SNS]_2$ metalloligand. **M. Wojnar**, A.F. Heyduk

PROF 35. Design, synthesis, applications of metabolic chemical reporters as tools for probing glycosylation pathways. **J. Moreno**, M. Pratt

PROF 36. Exploring the reactivity of actinide-pnictogen bonds. **S. Vilanova**, J.R. Walensky

Science of Sexual Harassment

Working to Stop Harassment in Departments & at Meetings

Sponsored by WCC, Cosponsored by PRES, PROF and YCC‡

Senior Chemists' Career Stories
Sponsored by SCHB, Cosponsored by PROF and SCC

Thriving in the Workplace: Non-Technical Skills that Boost your Value
Sponsored by BMGT, Cosponsored by PROF‡, SCHB, WCC‡ and YCC‡

Excellence in Graduate Polymer Research

Synthesis & New Materials

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY EVENING

Section A
Ernest N. Morial Convention Center

‡*Cooperative Cosponsorship*

Halls D/E

Sci-Mix
R. Libby, *Organizer*

8:00–10:00

25-36. See previous listings.

TUESDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 22

Ethics in Industry Collaborations that Work
Cosponsored by SCHB
S.M. Schelble, *Organizer*
P.A. Mabrouk, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 PROF 37. Corporate intersection of ethics and biotechnology. **R. Dhanda**

9:05 PROF 38. Ethics and forensic science. **T. DeAngelo**

9:35 PROF 39. Molecular mechanisms of ethical design. **J.C. Warner**

10:05 Intermission.

10:20 PROF 40. Preparing the next generation of molecular designers to practice greener chemistry through cross-sector partnerships. **A.S. Cannon**

10:50 PROF 41. Innovative training to reinforce a speak-up corporate culture: Voicing our values. **B. Marks**

11:20 Panel Discussion.

11:35 Concluding Remarks.

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Jani C. Ingram

Sponsored by ANYL, Cosponsored by PROF and WCC

Chemists & Writing for Fun & Profit: Write Your Own Career
Sponsored by SCHB, Cosponsored by BIOL and PROF

ACS Award for Encouraging Women into Careers in the Chemical Sciences

Symposium in Honor of Rebecca Ruck

Sponsored by WCC, Cosponsored by ORGN, PROF and YCC‡

Remarkable Women of Medicinal Chemistry
Sponsored by MEDI, Cosponsored by PROF and WCC

Excellence in Graduate Polymer Research

Bio-Related Polymers

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon D Sec 22

Chemistry Students at the Nexus: REU Award Winners
Cosponsored by CHED
K.L. Buchmueller, L.M. Watkins, *Organizers*

S.A. France, *Presiding*

1:30 Introductory Remarks.

1:35 PROF 42. Structural analysis of TCPP nanostructures. **T. Reyes**, M.B. Elinski, J.D. Batteas

1:50 PROF 43. Hybridizing self-assembling peptides with conductive polymers for biomedical applications. **L. Jenkins**, E.I. James, A. Murphy

2:05 PROF 44. Synthesis of antibacterial polymers. **S.D. Kendrick**, S. Sharpes, K. Seifert, K.L. Caran

2:20 PROF 45. Conformational analysis of furan and thiophene oligomers. **M. Webb**, T.L. Ellington, G.S. Tschumper

2:35 PROF 46. Determination of valuable metals in fracking waters. **M. Young**, B. Nespor, A. LaVallie, D.T. Pierce, M. Mann, Y. Wang, D. Laudal

2:50 Intermission.

3:10 PROF 47. Copper distribution in the cytoplasm of *Pseudomonas aeruginosa*. **G. Becker**, L. Novoa-Aponte, J. Argüello

3:25 PROF 48. Mild synthesis of a novel boron-based pharmaceutical candidate by copper catalysis with CO_2. **N. Ziemer**, T.M. Perrone, S. Knowlden, B.V. Popp

3:40 PROF 49. Predicting biomolecular diffusion using surface residue exposure. **J. Haseleu**, C. Fennell

3:55 PROF 50. Complexation of Hg(II) and Cd(II) with rhodizonate and nitrogen donor ligands. **S. Saluga**, J.A. Silverman, K. Kavallieratos

4:10 PROF 51. Synthesis of NU-1000 nanoparticles. **S. Bingham**, T. Webber, R. Penn

4:25 Concluding Remarks.

Science & Ethics: The Path Toward Global Security in Chemicals, Energy, Food & Water
Sponsored by SCHB, Cosponsored by CHAS, COMSCI, MPPG and PROF

WCC Rising Star Award Symposium
Sponsored by WCC, Cosponsored by BIOT, CHED, COLL, INOR and PROF

Excellence in Graduate Polymer Research

New Products & Characterization

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY EVENING

Excellence in Graduate Polymer Research
Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

SCHB

Division of Small Chemical Businesses

J. Sabol, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

BIOT Tank (see *BIOT*, Sun)

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of Javier Garcia Martinez (see *ENFL*, Tue, Wed)

Issues in Chemical Commercialization (see *CHAL*, Mon)

Thriving in the Workplace: Non-Technical Skills that Boost your Value (see *BMGT*, Mon)

SOCIAL EVENTS:

Reception, 6:30 PM: Mon

Coffee & Networking, 8:30 AM & 7:45 AM: Mon, Tue

Speakers' & Members' Luncheon, 11:30 AM: Tue

BUSINESS MEETINGS:

Business Meeting, 7:00 PM: Sat

Executive Committee Meeting, 7:15 PM: Sat

SUNDAY MORNING

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

SUNDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 15

Legal Issues for Chemical Companies in the Food, Energy & Water Industries
Cosponsored by CHAL and PROF
T. Siepmann, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 SCHB 1. Immigration issues facing chemists and chemical businesses. **B.H. Getson**

2:15 SCHB 2. Toxic Substances Control Act issues for chemical businesses in the food, energy, and water sectors. **I. Hantman**

2:55 SCHB 3. Getting the right starting material: Due diligence in the formation or acquisition of a chemical enterprise. **R.G. Hanshaw**

3:35 Intermission.

3:50 SCHB 4. Intellectual property and the clean energy sector. **S. Barkley**

4:30 SCHB 5. Trademark issues for chemical businesses in the food, energy,

and water sectors. **K.B. Drake**

5:10 Concluding Remarks.

Chemical Angel Network (CAN): Chemists Investing in Chemistry-Based Companies
Sponsored by BMGT, Cosponsored by PROF and SCHB‡

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

SUNDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls B2/C

Entrepreneurs' Poster Session
Cosponsored by PROF
G.W. Ruger, *Organizer*

6:00–8:00

SCHB 6. Learn how SCHB assists innovators and entrepreneurs in the chemistry enterprise. **P.C. Lauro**, **M. Chorghade**, **A. Kantak**, **D.J. Deutsch**, **J.E. Sabol**, **J.L. Maclachlan**, **C.A. Burton**, **E.L. Oltermann**, **J.L. Bryant**, **T. Siepmann**, **G.W. Ruger**, **P.J. Bonk**, **R. Chorghade**, **N.A. Vaidya**, **A. Rahman**

SCHB 7. Chemical Angel Network: Chemical professionals investing in chemistry enabled businesses. **S.S. White**, M. Vreeke, J.C. Giordan

SCHB 8. Template for industry outreach collaboration in Lehigh Valley, Pennsylvania. **J.R. Berk**, **G.W. Ruger**

SCHB 9. Design of capacitive water treatment systems for preferential ion removal. L. Boehme, **J. Landon**, C. Lippert

MONDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 15

Public Policy in Food, Energy & Water Issues
Cosponsored by CCPA
Financially supported by Saul Ewing LLP
J.E. Sabol, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 SCHB 10. Public policy issues in food, energy, and water. **A. Pitagno**, **D. Nierenberg**, **P.R. Robinson**, **V.V. Rajasekharan**

10:05 SCHB 11. Panel discussion on public policy issues in food, energy, and water. **A. Pitagno**, **D. Nierenberg**, **P.R. Robinson**, **V.V. Rajasekharan**

Women in Cannabis: Shaping an Emerging Industry
Sponsored by CHAS, Cosponsored by SCHB‡ and WCC

MONDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 15

Senior Chemists' Career Stories
Cosponsored by PROF and SCC
E. Meyer, *Organizer*
J.E. Sabol, *Organizer, Presiding*

1:25 Introductory Remarks.

1:30 SCHB 12. From academic laboratory to commercialization: The ThruPore story. **M.G. Bakker**

1:55 SCHB 13. Encounters with two past ACS presidents. **E. Meyer**

2:20 SCHB 14. A year in the life of an ACS president. **E.A. Nalley**

2:45 SCHB 15. Building Alchemie: An educational technology company from a chemistry classroom. **J. Winter**

3:10 Intermission.

3:20 SCHB 16. I never intended to teach: An outline of a non-linear career path. **L.G. Hartshorn**

3:45 SCHB 17. Career for chemists in sales, marketing, and management. **J.P. Stoner**

4:10 SCHB 18. Two lives: Chemist and ACS president. **A.E. Pavlath**

4:35 SCHB 19. From the bench to the bench: perspectives on a career from the laboratory to the courtroom. **P.C. Lauro**

Thriving in the Workplace: Non-Technical Skills that Boost your Value
Sponsored by BMGT, Cosponsored by PROF‡, SCHB, WCC‡ and YCC‡

MONDAY EVENING

Section A
Ernest N. Morial Convention Center
Halls D/E

Sci-Mix
G.W. Ruger, *Organizer*

8:00–10:00

6-9. See previous listings.

TUESDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 15

Chemists & Writing for Fun & Profit: Write Your Own Career
Cosponsored by BIOL and PROF
Financially supported by Saul Ewing LLP
L.M. Balbes, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 SCHB 20. Communication solved, or how my grandparents learned to love synthetic organic chemistry. **T.N. Hoerter**

9:05 SCHB 21. Never mistake an e-mail with reality (or the importance of writing well). **A.M. Noce**

9:35 SCHB 22. Proposals and blogging and books, oh my. **M.R. Hartings**

10:05 Intermission.

10:20 SCHB 23. Practical notes: Developing a writing practice as a working chemist. **M.M. Francl**

10:50 SCHB 24. No education of any kind is ever wasted. **H.J. Elston**

11:20 SCHB 25. On column detection. **R.M. Burks**

Ethics in Industry Collaborations that Work
Sponsored by PROF, Cosponsored by SCHB

TUESDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 15

Science & Ethics: The Path Toward Global Security in Chemicals, Energy, Food & Water
Cosponsored by CHAS, COMSCI, MPPG and PROF
J.L. Bryant, *Organizer*
K. Rodda, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 SCHB 26. IUPAC, ethics, and chemical safety and security. **M.C. Cesa**

2:00 SCHB 27. Industrial perspective: Synergies between industrial security and ethics. **D. Hupaylo**

2:25 SCHB 28. Chemical security multipliers: securing global chemical weapons assets through international capacity building initiatives. **T. Brown**

2:50 Intermission.

3:10 SCHB 29. Global Chemists' Code of Ethics. **L. Brown**

3:35 SCHB 30. Incentives for small chemical companies' adoption of ethical codes: key components in the prevention of reemergence of chemical weapons. **K. Rodda**

4:00 SCHB 31. Path toward global security in biotechnology and synthetic biology research. **K.M. Omberg**

4:25 Concluding Remarks.

WEDNESDAY MORNING

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Sponsored by CHAS, Cosponsored by AGFD, CHAL and SCHB

WEDNESDAY AFTERNOON

Heidolph North America's Cannabis Chemistry Subdivision Scholarship Symposium
Sponsored by CHAS, Cosponsored by AGFD, CHAL and SCHB

CCS

Committee on Chemical Safety

R. Stuart, *Program Chair*

SUNDAY AFTERNOON

Ask Dr. Safety: Integrating Research & Safety
Sponsored by CHAS, Cosponsored by CCS

MONDAY AFTERNOON

Implementing ACS Safety Education Guidelines
Sponsored by CHAS, Cosponsored by CCS and CHED

TUESDAY MORNING

Water Supply Safety
Sponsored by CHAS, Cosponsored by CCS, CTA and ENVR

CCPA

Committee on Chemistry & Public Affairs

R. Forslund, *Program Chair*

MONDAY MORNING

Public Policy in Food, Energy & Water Issues
Sponsored by SCHB, Cosponsored by CCPA

CWD

Committee on Chemists with Disabilities

L. Hoffman, *Program Chair*

SUNDAY MORNING

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY AFTERNOON

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

MONDAY AFTERNOON

LGBTQ+ Graduate Student &

‡*Cooperative Cosponsorship*

Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

CCA

Committee on Community Activities

M. McGinnis, *Program Chair*

WEDNESDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

WEDNESDAY AFTERNOON

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

THURSDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

CORP

Committee on Corporation Associates

D.G. Schmidt, *Program Chair*

MONDAY MORNING

Community Sharing of Chemical Safety Data: Yes, No, Maybe?
Sponsored by CINF, Cosponsored by CHAS, CORP and PRES‡

DAC

Committee on Divisional Activities

R. Bennett, *Program Chair*

SUNDAY MORNING

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Membranes for Water & Ion Transport

Sponsored by PMSE, Cosponsored by DAC‡

SUNDAY AFTERNOON

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Novel Membranes & Membrane Functionalization

Sponsored by PMSE, Cosponsored by DAC‡

MONDAY MORNING

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Membranes for Gas & Small-Molecule Separations

Sponsored by PMSE, Cosponsored by DAC‡

MONDAY AFTERNOON

Food at the Crossroads: Chemistry's Role in Sustainability, Past & Present
Sponsored by HIST, Cosponsored by AGFD, CHED, DAC‡, MPPG‡ and PRES‡

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

Biofouling & Bioseparations

Sponsored by PMSE, Cosponsored by DAC‡

TUESDAY MORNING

PMSE-North American Membrane Society (NAMS) Joint Symposium on Surface Science of Membranes for Advanced Separations

MOFs & 2D Membrane Materials

Sponsored by PMSE, Cosponsored by DAC‡

CEI

Committee on Environmental Improvement

C. Middlecamp, *Program Chair*

SUNDAY MORNING

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

Citizens First!
Sponsored by CHED, Cosponsored by CEI

SUNDAY AFTERNOON

Citizens First!
Sponsored by CHED, Cosponsored by CEI

Perspectives on Climate Change Literacy & Education: Local to International
Sponsored by CHED, Cosponsored by CEI

MONDAY MORNING

ACS-CEI Award for Incorporating Sustainability into Chemical Education
Sponsored by CHED, Cosponsored by CEI and ENVR

Innovative Chemical & Material Approaches for Sustainable Water Purification

Adsorption

Sponsored by ENVR, Cosponsored by CEI

MONDAY AFTERNOON

Innovative Chemical & Material Approaches for Sustainable Water Purification

Electrochemistry & Membrane Technology

Sponsored by ENVR, Cosponsored by CEI

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern
Sponsored by ENVR, Cosponsored by ANYL and CEI

Undergraduate Research Posters

Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by CEI and SOCED

TUESDAY MORNING

Innovative Chemical & Material Approaches for Sustainable Water Purification

Photocatalysis

Sponsored by ENVR, Cosponsored by CEI

Green Chemistry Theory & Practice: Food, Energy & Water Sustainability
Sponsored by CHED, Cosponsored by CEI

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern
Sponsored by ENVR, Cosponsored by CEI

TUESDAY AFTERNOON

Science & its Perception: Climate Change, Nicotine, Pollution & Other Emerging Topics in the Crosshair
Sponsored by ENVR, Cosponsored by CEI‡

Innovative Chemical & Material Approaches for Sustainable Water Purification

Oxidation & Sensor

Sponsored by ENVR, Cosponsored by CEI

Green Chemistry Theory & Practice: Food, Energy & Water Sustainability
Sponsored by CHED, Cosponsored by CEI

Ongoing Challenges in the Treatment of Contaminants of Emerging Concern
Sponsored by ENVR, Cosponsored by CEI

WEDNESDAY MORNING

Current State of Environmental Contamination Research: Theory & Experiment
Sponsored by ENVR, Cosponsored by CEI

Innovative Chemical & Material Approaches for Sustainable Water Purification

Catalysis

Sponsored by ENVR, Cosponsored by CEI

WEDNESDAY AFTERNOON

Current State of Environmental Contamination Research: Theory & Experiment
Sponsored by ENVR, Cosponsored by CEI

Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery
Sponsored by ENVR, Cosponsored by CEI

THURSDAY MORNING

Green Chemistry & the Environment
Sponsored by ENVR, Cosponsored by CEI

Current State of Environmental Contamination Research: Theory & Experiment
Sponsored by ENVR, Cosponsored by CEI

Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery
Sponsored by ENVR, Cosponsored by CEI

THURSDAY AFTERNOON

Current State of Environmental Contamination Research: Theory & Experiment
Sponsored by ENVR, Cosponsored by CEI

Emerging Environmental Biotechnologies for Energy-Efficient Pollutant Control, Remediation & Resource Recovery
Sponsored by ENVR, Cosponsored by CEI

LSAC

Committee on Local Section Activities

J. Ritchie, *Program Chair*

WEDNESDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

WEDNESDAY AFTERNOON

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

THURSDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

‡*Cooperative Cosponsorship*

CMA

Committee on Minority Affairs

J. Sarquis, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium (see *PROF*, Sun, Mon)

SOCIAL EVENTS:

Social Hour, 5:00 PM: Sun

Luncheon, 11:30 AM: Mon

BUSINESS MEETINGS:

Business Meeting, 7:30 AM: Sun

SUNDAY MORNING

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY AFTERNOON

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

MONDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon B Sec 7

How to Foster Diversity in the Chemical Sciences

Lessons Learned & Taught Through the Stories of Recipients of the Stanley C. Israel Award

Cosponsored by PROF and WCC
J.L. Sarquis, *Organizer*
D. Afzal, R. Joseph, *Organizers, Presiding*

8:00 Introductory Remarks.

8:05 CMA 1. Supporting university and K-12 students through outreach program. **S.J. Olesik**, J. Caton

8:25 CMA 2. Success in mentoring and training minority undergraduate scientists to Ph.D. degrees. **K.H. Pannell**

8:45 CMA 3. Diversity and inclusion in chemistry teaching and research: Some personal challenges and opportunities. **D. Rabinovich**

9:05 CMA 4. Nine years in the Midwest: A new beginning? **J. Vela**

9:25 Intermission.

9:40 CMA 5. Diversity and excellence: Advice for department chairmen. **J.V. Ortiz**

10:00 CMA 6. The Alliance for Diversity in Science and Engineering: Empowering graduate students. **S.A. Lopez**

10:20 CMA 7. Diversity: The key to excellence in chemistry. **E.A. Nalley**

10:40 CMA 8. My path for fostering diversity. **Z.C. Morales Martinez**

11:00 Concluding Remarks.

MONDAY AFTERNOON

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

CPRC

Committee on Public Relations & Communications

J. Mcclachlan, *Program Chair*

SUNDAY AFTERNOON

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

COMSCI

Committee on Science

M. Fisher, *Program Chair*

TUESDAY AFTERNOON

Science & Ethics: The Path Toward Global Security in Chemicals, Energy, Food & Water
Sponsored by SCHB, Cosponsored by CHAS, COMSCI, MPPG and PROF

SCC

Senior Chemists Committee

T. Beattie, *Program Chair*

MONDAY AFTERNOON

Senior Chemists' Career Stories
Sponsored by SCHB, Cosponsored by PROF and SCC

SOCED

Society Committee on Education

N. Bastian, *Program Chair*

EVENTS:

Where Can My Chemistry Degree Take Me? 9:30 AM: Sun

Chem Demo Exchange, 11:00 AM: Sun

Grad School Fair, 1:00 PM: Sun

ACS Student Chapter Awards Ceremony, 7:00 PM: Sun

ACS Undergraduate Social, 8:30 PM: Sun

The Chemistry that Keeps America Safe, 10:00 AM: Mon

SUNDAY MORNING

Chemistry Teachers Day Program
Sponsored by CHED, Cosponsored by SOCED

SUNDAY AFTERNOON

Chemistry Teachers Day Program
Sponsored by CHED, Cosponsored by SOCED

MONDAY MORNING

Excellence in Graduate Polymer Research

Polymerization Techniques

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Section A
Ernest N. Morial Convention Center
Rooms 356/357

Eminent Scientist Lecture with Dr. Mary Jo Ondrechen

N. R. Bastian, *Organizer, Presiding*

2:30 Introductory Remarks.

2:40 SOCED 1. Thinking outside the informatics box: Concepts from chemistry for understanding genomes. **M.J. Ondrechen**

3:40 Q&A.

3:55 Concluding Remarks.

Excellence in Graduate Polymer Research

Synthesis & New Materials

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Undergraduate Research Posters

Agricultural & Food Chemistry

Sponsored by CHED, Cosponsored by AGFD and SOCED

Undergraduate Research Posters

Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

Undergraduate Research Posters

Biotechnology

Sponsored by CHED, Cosponsored by BIOT and SOCED

Undergraduate Research Posters

Chemical Education

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

Undergraduate Research Posters

Environmental Chemistry

Sponsored by CHED, Cosponsored by ENVR and SOCED

Undergraduate Research Posters

Geochemistry

Sponsored by CHED, Cosponsored by GEOC and SOCED

Undergraduate Research Posters

Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by CEI and SOCED

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

Undergraduate Research Posters

Nanochemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Organic Chemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Physical Chemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

TUESDAY MORNING

Excellence in Graduate Polymer Research

‡*Cooperative Cosponsorship*

Bio-Related Polymers

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

TUESDAY AFTERNOON

Excellence in Graduate Polymer Research

New Products & Characterization

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

TUESDAY EVENING

Excellence in Graduate Polymer Research
Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

WEDNESDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

WEDNESDAY AFTERNOON

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

THURSDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

THURSDAY AFTERNOON

Polymer Networks: Soft Gels to Stiff Networks
Sponsored by POLY, Cosponsored by PHYS, PMSE and SOCED

CTA

Committee on Technician Affairs

C. Libby, *Program Chair*

SUNDAY MORNING

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

SUNDAY AFTERNOON

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

TUESDAY MORNING

Water Supply Safety
Sponsored by CHAS, Cosponsored by CCS, CTA and ENVR

WCC

Women Chemists Committee

R. Cole, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

How to Foster Diversity in the Chemical Sciences (see *CMA*, Mon)

Thriving in the Workplace: Non-Technical Skills that Boost your Value (see *BGMT*, Mon)

Women in Cannabis: Shaping an Emerging Industry (see *CHAS*, Mon)

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Jani C. Ingram (see *ANYL*, Tue)

Remarkable Women of Medicinal Chemistry (see *MEDI*, Tue)

SUNDAY MORNING

E.V. Murphree Award in Industrial and Engineering Chemistry: Symposium in honor of Linda J. Broadbelt
Sponsored by I&EC, Cosponsored by WCC

Earle B. Barnes Award for Leadership in Chemical Research Management: Symposium in honor of Margaret M. Faul
Sponsored by ORGN, Cosponsored by WCC

Synthetic Chemistry Addressing Challenges in Energy & the Environment
Sponsored by INOR, Cosponsored by CATL and WCC

ACS Award in Applied Polymer Science: Symposium in honor Paula T. Hammond
Sponsored by PMSE, Cosponsored by POLY and WCC

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Sponsored by INOR, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Atomic-Level Precision in Deposition & Etching
Sponsored by COLL, Cosponsored by WCC

SUNDAY AFTERNOON

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Synthetic Chemistry Addressing Challenges in Energy & the Environment
Sponsored by INOR, Cosponsored by CATL and WCC

ACS Award in Applied Polymer Science: Symposium in honor Paula T. Hammond
Sponsored by PMSE, Cosponsored by POLY and WCC

E.V. Murphree Award in Industrial and Engineering Chemistry: Symposium in honor of Linda J. Broadbelt
Sponsored by I&EC, Cosponsored by WCC

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Sponsored by INOR, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Nanomaterials & Catalysis on the Nanoscale
Sponsored by COLL, Cosponsored by WCC

SUNDAY EVENING

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Sponsored by INOR, Cosponsored by WCC

MONDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 13

Science of Sexual Harassment

The Psychology & Sociology of Sexual Harassment

Cosponsored by PRES, PROF and YCC‡
Financially supported by C&EN
S. Azad, S.R. Hare, A. Widener, *Organizers*
L. Wang, *Organizer, Presiding*

9:00 WCC 1. Sexual harassment on college campuses. **S. Sun**

9:15 WCC 2. The whys and hows of sexual harassment: What organizations should be doing. **V. Magley**

9:35 WCC 3. Gender salience and racial frames, potential potholes for women in science: Understanding the context before and the potential consequences of sexual harassment. **E. Branch**

9:55 Intermission.

10:05 WCC 4. The cost of cosmetic. **J. Grossman**

10:25 WCC 5. From the personal to the profession: Steps we must take to end sexual harassment. **M. Boyd**

10:45 Panel Discussion.

How to Foster Diversity in the Chemical Sciences

Lessons Learned & Taught Through the Stories of Recipients of the Stanley C. Israel Award
Sponsored by CMA, Cosponsored by PROF and WCC

Women in Cannabis: Shaping an Emerging Industry
Sponsored by CHAS, Cosponsored by SCHB‡ and WCC

Ralph F. Hirschmann Award in Peptide Chemistry: Symposium in honor of Lila M. Gierasch

Bridging Peptides & Proteins: From Function to Therapy

Sponsored by BIOL, Cosponsored by WCC

E.V. Murphree Award in Industrial and Engineering Chemistry: Symposium in honor of Linda J. Broadbelt
Sponsored by I&EC, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Surface Modification & Function

Sponsored by COLL, Cosponsored by WCC

MONDAY AFTERNOON

‡*Cooperative Cosponsorship*

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 13

Science of Sexual Harassment

Working to Stop Harassment in Departments & at Meetings

Cosponsored by PRES, PROF and YCC‡
Financially supported by C&EN
S. Azad, L. Wang, A. Widener, *Organizers*
S.R. Hare, *Organizer, Presiding*

1:00 WCC 6. Taking back my power: My story of sexual harassment. **M. Dulay**

1:15 WCC 7. Mediating sexual harassment issues in science. **N. Frank**

1:35 WCC 8. Redefining expectations: The role for scientific societies in addressing harassment in science and other work climate issues. **B.M. Williams**

1:55 Intermission.

2:05 WCC 9. Preventing sexual harassment: Some experiences with a program aimed at graduate students, faculty, and staff. **N. Giordano**

2:25 WCC 10. GRC Power Hour: Culture-change begins at the frontiers of science. **N.R. Gray**

2:45 Panel Discussion.

Thriving in the Workplace: Non-Technical Skills that Boost your Value
Sponsored by BMGT, Cosponsored by PROF‡, SCHB, WCC‡ and YCC‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

James Flack Norris Award in Physical Organic Chemistry: Symposium in honor of Cynthia J. Burrows
Sponsored by ORGN, Cosponsored by WCC

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry: Symposium in honor of Alison Butler
Sponsored by INOR, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Interfaces & Assembly: From Molecular Understanding to 3D Materials

Sponsored by COLL, Cosponsored by WCC

TUESDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 13

ACS Award for Encouraging Women into Careers in the Chemical Sciences

Symposium in Honor of Rebecca Ruck

Cosponsored by ORGN, PROF and YCC‡
E.C. Sherer, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 WCC 11. Importance of mechanistic understanding towards process understanding. **Y. Ji Chen**

9:00 WCC 12. New synthetic opportunities with nitrones and hydroxamic acids. **L.L. Anderson**, M. Kroc, T. Reidl, J. Son

9:25 WCC 13. Stereocontrol in photochemical synthesis. **T.P. Yoon**

9:50 WCC 14. Accessing novel phosphoramidate prodrugs via the protecting-group free selective 3′-functionalization of nucleosides. **J. McCabe Dunn**, m. Reibarkh, E.C. Sherer, R. Orr, R. Ruck

10:15 Intermission.

10:25 WCC 15. From JANUVIA to MARIZEV (Omarigliptin), a once weekly DPP-4 inhibitor for the treatment of diabetes. **A.E. Weber**

10:50 WCC 16. Alkynes of transformations. **V.M. Dong**

11:15 WCC 17. Award Address (ACS Award for Encouraging Women into Careers in the Chemical Sciences Sponsored by The Camille and Henry Dreyfus Foundation, Inc.). Science, mentors, role models & more: The ongoing pursuit to inspire more women into successful chemistry careers. **R. Ruck**

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Jani C. Ingram
Sponsored by ANYL, Cosponsored by PROF and WCC

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Novel Materials Design

Sponsored by PMSE, Cosponsored by WCC

Remarkable Women of Medicinal Chemistry
Sponsored by MEDI, Cosponsored by PROF and WCC

George C. Pimentel Award in Chemical Education
Sponsored by CHED, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Stacey F. Bent

Atomic-Layer Deposition & its Applications

Sponsored by COLL, Cosponsored by WCC

TUESDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 13

WCC Rising Star Award Symposium
Cosponsored by BIOT, CHED, COLL, INOR and PROF
M.A. Kane, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 WCC 18. Materials chemistry for plastic batteries. **J.L. Lutkenhaus**

1:55 WCC 19. Unlocking the biotech potential of gut microbes from herbivores. **M.A. O'Malley**

2:15 WCC 20. Chemical Education Research and ACS Exams: How I discovered my passion that became my career. **K.L. Murphy**

2:35 Intermission.

2:50 WCC 21. Design and discovery of molecular modules for artificial photosynthesis. **K.L. Mulfort**

3:10 WCC 22. Collaboration and conformation in new drug discovery. **M. Machacek**

3:30 WCC 23. Maximizing impact through collaboration. **X. Chen**

3:50 Concluding Remarks.

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Advanced Structure Analysis

Sponsored by PMSE, Cosponsored by WCC

George C. Pimentel Award in Chemical Education
Sponsored by CHED, Cosponsored by WCC

ACS Award Symposium for Creative Advances in Environmental Science & Technology
Sponsored by ENVR, Cosponsored by WCC

WEDNESDAY MORNING

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Processing-Structure-Property Relationships

Sponsored by PMSE, Cosponsored by WCC

Upstream Processes

Synthetic Biology

Sponsored by BIOT, Cosponsored by WCC

General Papers: New Concepts in Polymeric Materials
Sponsored by PMSE, Cosponsored by WCC

WEDNESDAY AFTERNOON

ACS Award in the Chemistry of Materials: Symposium in honor of Elsa Reichmanis

Frontiers in Chemistry of Materials

Sponsored by PMSE, Cosponsored by WCC

YCC

Younger Chemists Committee

D. Williams, K. Heroux and M. Brann, *Program Chairs*

SUNDAY MORNING

Water, Water Everywhere But Not a Drop to Drink: Preserving, Protecting & Delivering Clean Water
Sponsored by PRES, Cosponsored by AGFD, BMGT, CATL, CEI, CELL, CHAS, CHED, COLL, CTA, ENVR, GEOC, I&EC, INOR, MPPG, SCHB and YCC

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Emerging Applications of Organic & Biochemistry: Soil Science, Biomaterials & Synthesis

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

SUNDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 18

Starting a Successful Research Program at a PUI
Cosponsored by PROF
M.L. Druelinger, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 YCC 1. Using undergraduate research to help shape STEM education. **M.R. Malachowski**

1:20 YCC 2. Collaborative research with undergraduates: Research project and research design. **A.M. Schoffstall**

1:40 YCC 3. Maintaining equilibrium between teaching, research, service and life at predominantly undergraduate institutions (PUIs). **B.L. Gourley**

2:00 YCC 4. Art and necessity of gaining internal support from institutional administrators. **M.L. Druelinger**

2:20 Intermission.

2:30 YCC 5. Undergraduate new investigator grants at the ACS Petroleum Research Fund. **T. Clancy**

2:55 YCC 6. Funding opportunities at the National Science Foundation of interest to faculty at primarily undergraduate institutions (PUIs). **S. Atlas**

3:25 YCC 7. Writing more competitive grant proposals. **M.R. Malachowski**

3:45 YCC 8. Finding small pockets of funding to jump-start your research. **B.L. Gourley**

4:05 Panel Discussion.
4:25 Concluding Remarks.

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium

Experimental & Computational Frontiers in Inorganic & Materials Chemistry

‡*Cooperative Cosponsorship*

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, BIOT, CHED, CMA, COLL, COMP‡, CWD, ENVR, INOR‡, MEDI‡, ORGN, PHYS‡, PMSE‡, POLY‡, PRES‡, WCC and YCC

Science Cafes & Engaging the Public: Techniques for Hosting Successful Events
Sponsored by PRES, Cosponsored by CATL, CELL, CHAS, CHED, COLL, CPRC, CTA, ENVR, I&EC, INOR, MPPG, SCHB and YCC

MONDAY MORNING

Section A
Hilton New Orleans Riverside
Grand Ballroom D

Molecules that Changed the World
Cosponsored by HIST and I&EC
M. Grandbois, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 YCC 9. Enabling Moore's Law through chemistry. **P. Trefonas**, J.F. Cameron, J.W. Thackeray, M. Li

9:35 YCC 10. Perspectives on agrochemical discovery. **B.A. Lorsbach**, T.C. Sparks

10:05 YCC 11. Advances in olefin block copolymers. **D.M. Pearson**

10:35 Intermission.

10:50 YCC 12. Development for fluorolefins for refrigeration. **R. Singh**

11:20 YCC 13. Race to cleaner air: How cordierite revolutionized the automotive industry. **D.M. Beall**

11:50 Concluding Remarks.

Science of Sexual Harassment

The Psychology & Sociology of Sexual Harassment

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Excellence in Graduate Polymer Research

Polymerization Techniques

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Ballroom D

Tales of Chemistry & Cocktails
Cosponsored by HIST
Financially supported by C&EN
J. Schwarzbach, *Organizer*
K.J. Heroux, *Organizer, Presiding*
L.K. Wolf, *Presiding*

2:00 Introductory Remarks.

2:05 YCC 14. Cocktails: Study your senses before you dull them. **M.R. Hartings**

2:30 YCC 15. Getting into sloe business. **S.J. Cantrill**

2:55 YCC 16. Beer, a bordello, and a barrister. **R.M. Burks**

3:20 Intermission.
3:25 Panel Discussion.

Science of Sexual Harassment

Working to Stop Harassment in Departments & at Meetings

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Thriving in the Workplace: Non-Technical Skills that Boost your Value
Sponsored by BMGT, Cosponsored by PROF‡, SCHB, WCC‡ and YCC‡

LGBTQ+ Graduate Student & Postdoctoral Scholar Research Symposium
Sponsored by PROF, Cosponsored by ANYL, BIOL, BIOT, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, ORGN, PHYS, PMSE, POLY, WCC and YCC

Excellence in Graduate Polymer Research

Synthesis & New Materials

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TUESDAY MORNING

ACS Award for Encouraging Women into Careers in the Chemical Sciences

Symposium in Honor of Rebecca Ruck

Sponsored by WCC, Cosponsored by ORGN, PROF and YCC‡

Excellence in Graduate Polymer Research

Bio-Related Polymers

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TUESDAY AFTERNOON

Section A
Hilton New Orleans Riverside
Grand Salon C Sec 18

Young Chemists & Water
Cosponsored by PHYS
N. Hammer, J.T. Kelly, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 YCC 17. Probing hydrogen bonding in Nitrogen-containing heterocyclic molecules using Raman under nitrogen spectroscopy. **T. Powell**, K. Stevens, J.T. Kelly, N. Hammer

1:25 YCC 18. Theoretical approaches for treating non-valence correlation-bound anions. **A. Kairalapova**, K.D. Jordan

1:45 YCC 19. Water world: Understanding water's diverse interactions with solutes through single-conformation spectroscopy. **P.S. Walsh**, D.P. Tabor, R. Kusaka, E.G. Buchanan, J. Gord, E.L. Sibert, T.S. Zwier

2:10 YCC 20. Probing the energetics and vibrational signatures of the azide-water complex. **T.L. Ellington**, J.T. Kelly, T.M. Sexton, R.C. Fortenberry, K.R. Asmis, G.S. Tschumper

2:30 Intermission.

2:45 YCC 21. Ions in water: A microscopic look at microhydration. **J.T. Kelly**, K.R. Asmis

3:10 YCC 22. Intrinsic energetics of proton transfer in binary $(HF)_m(H_2O)_n$ and $(HCl)_m(H_2O)_n$ clusters. **S.N. Johnson**, G.S. Tschumper

3:30 YCC 23. Intermolecular interactions between TMAO and water: Restructuring the water hydrogen bonding network. **L.E. McNamara**, H.U. Valle, F.R. Fronczek, T.K. Hollis, G.S. Tschumper, N. Hammer

3:50 YCC 24. One-dimensional adiabatic models for the coupling of low-frequency intermolecular modes with OH stretch modes in water-ion clusters. **B. Henderson**, K.D. Jordan

4:10 YCC 25. Unraveling the spectroscopic signatures of divalent metal ion binding to carboxylate head groups at the air-water interface with cold gas-phase clusters. **J.K. Denton**, P.J. Kelleher, J. DePalma, H.C. Allen, C.J. Mundy, M.A. Johnson

4:35 YCC 26. Dual cryogenic ion trap spectroscopy for the formation and characterization of solvated peptides. **J.M. Voss**, K. Fischer, B. Marsh, E. Garand

Excellence in Graduate Polymer Research

New Products & Characterization

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TUESDAY EVENING

Excellence in Graduate Polymer Research
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WEDNESDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

WEDNESDAY AFTERNOON

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

THURSDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment
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‡*Cooperative Cosponsorship*

Wang, S.	POLY	331	**Wang, X.**	GEOC	270	**Wang, Y.**	I&EC	90
Wang, S.	POLY	534	**Wang, X.**	CELL	228	**Wang, Y.**	PMSE	299
Wang, S.	POLY	535	**Wang, X.**	MPPG	9	**Wang, Y.**	INOR	750
Wang, S.	ENVR	182	**Wang, X.**	INOR	575	**Wang, Y.**	PHYS	620
Wang, S.	ENVR	486	**Wang, X.**	INOR	1154	**Wang, Y.**	PMSE	175
Wang, S.	BIOT	23	**Wang, X.**	INOR	1245	**Wang, Y.**	PMSE	364
Wang, S.	I&EC	31	**Wang, X.**	BIOL	195	**Wang, Y.**	MEDI	75
Wang, S.	COMP	243	**Wang, X.**	CATL	488	**Wang, Y.**	COLL	149
Wang, S.	INOR	1030	**Wang, X.**	ENFL	512	**Wang, Y.**	POLY	465
Wang, S.	CARB	43	**Wang, X.**	ENVR	83	**Wang, Y.**	ORGN	81
Wang, S.	ENFL	541	**Wang, X.**	ENVR	85	**Wang, Y.**	POLY	286
Wang, S.	BIOL	184	**Wang, X.**	GEOC	42	**Wang, Y.**	PMSE	555
Wang, S.	CATL	23	**Wang, X.**	CELL	218	**Wang, Y.**	POLY	633
Wang, S.	COMP	95	**Wang, X.**	MEDI	366	**Wang, Y.**	GEOC	239
Wang, S.	ENVR	157	**Wang, X.**	PMSE	593	**Wang, Y.**	BIOL	285
Wang, S.	AGFD	58	**Wang, X.**	INOR	750	**Wang, Y.**	COMP	340
Wang, S.	INOR	737	**Wang, X.**	ENFL	346	**Wang, Y.**	ENVR	773
Wang, S.	INOR	552	**Wang, X.**	BIOT	154	**Wang, Y.**	INOR	161
Wang, T.	CATL	102	**Wang, X.**	CELL	208	**Wang, Y.**	PROF	46
Wang, T.	ENFL	211	**Wang, X.**	FLUO	36	**Wang, Y.**	INOR	723
Wang, T.	ORGN	171	**Wang, X.**	ANYL	221	**Wang, Y.**	CATL	543
Wang, T.	ORGN	354	**Wang, X.**	MEDI	117	**Wang, Y.**	ENFL	47
Wang, T.	PMSE	368	**Wang, X.**	CATL	455	**Wang, Y.**	PMSE	354
Wang, T.	PMSE	448	**Wang, Y.**	BIOT	211	**Wang, Z.**	PMSE	529
Wang, T.	INOR	789	**Wang, Y.**	BIOT	213	**Wang, Z.**	CATL	455
Wang, T.	INOR	1236	**Wang, Y.**	ENVR	141	**Wang, Z.**	ORGN	607
Wang, T.	AGFD	64	**Wang, Y.**	ORGN	564	**Wang, Z.**	ENVR	187
Wang, T.	ENVR	588	**Wang, Y.**	CATL	186	**Wang, Z.**	CELL	38
Wang, T.	ENFL	355	**Wang, Y.**	ENFL	186	**Wang, Z.**	COMP	404
Wang, T.	INOR	716	**Wang, Y.**	ENFL	541	**Wang, Z.**	ANYL	450
Wang, T.	INOR	1422	**Wang, Y.**	ENVR	88	**Wang, Z.**	CHED	430
Wang, T.C.	INOR	432	**Wang, Y.A.**	PHYS	48	**Wang, Z.**	CHED	446
Wang, T.	I&EC	96	**Wang, Y.**	CATL	541	**Wang, Z.**	CHED	1027
Wang, T.	POLY	27	**Wang, Y.**	COMP	196	**Wang, Z.**	CHED	1029
Wang, T.	CELL	1	**Wang, Y.**	AGFD	213	**Wang, Z.**	CHED	1269
Wang, W.	ENVR	692	**Wang, Y.**	CATL	114	**Wang, Z.**	ENFL	175
Wang, W.	I&EC	116	**Wang, Y.**	ENFL	85	**Wang, Z.**	INOR	345
Wang, W.	POLY	330	**Wang, Y.**	I&EC	10	**Wang, Z.**	ENVR	406
Wang, W.	AGFD	213	**Wang, Y.**	MEDI	66	**Wang, Z.**	MEDI	277
Wang, W.	INOR	619	**Wang, Y.**	GEOC	28	**Wang, Z.**	INOR	756
Wang, W.	COLL	578	**Wang, Y.**	CATL	67	**Wang, Z.**	MEDI	19
Wang, W.	COLL	586	**Wang, Y.**	I&EC	13	**Wang, Z.**	ENFL	26
Wang, W.	COLL	607	**Wang, Y.**	ENVR	135	**Wang, Z.**	CATL	460
Wang, W.	PHYS	384	**Wang, Y.**	ENVR	275	**Wang, Z.**	CHED	171
Wang, W.	ENVR	326	**Wang, Y.**	ENVR	395	**Wang, Z.**	COLL	54
Wang, W.	MEDI	332	**Wang, Y.**	ENFL	48	**Wang, Z.**	ENVR	681
Wang, W.	INOR	786	**Wang, Y.**	ENFL	416	**Wang, Z.L.**	ANYL	411
Wang, X.	CATL	3	**Wang, Y.**	ENVR	25	**Wang, Z.**	COLL	416
Wang, X.	ORGN	377	**Wang, Y.**	INOR	1066	**Wang, Z.**	ENVR	57
Wang, X.	CELL	73	**Wang, Y.**	ORGN	303	**Wang, Z.**	CATL	475
Wang, X.	MEDI	294	**Wang, Y.**	PHYS	115	**Wang, Z.**	ENFL	68
Wang, X.	ORGN	538	**Wang, Y.**	ANYL	364	**Wang, Z.**	INOR	489
Wang, X.	ENVR	84	**Wang, Y.**	CATL	67	**Wang, Z.**	ENFL	34
Wang, X.	ENVR	724	**Wang, Y.**	CATL	293	**Wang, Z.**	COLL	734
Wang, X.	GEOC	243	**Wang, Y.**	I&EC	36	**Wang, Z.**	ENFL	106

Zhang, P.	ENFL	361	**Zhang, T.**	PHYS	424	**Zhang, X.**	POLY	36
Zhang, P.	ENVR	748	**Zhang, T.**	ENVR	11	**Zhang, X.**	POLY	425
Zhang, P.	PHYS	140	**Zhang, T.**	ENVR	204	**Zhang, X.**	INOR	831
Zhang, P.	PHYS	437	**Zhang, T.**	ENVR	453	**Zhang, X.**	BIOL	228
Zhang, P.	CATL	535	**Zhang, T.**	INOR	54	**Zhang, X.**	INOR	566
Zhang, P.	INOR	1404	**Zhang, V.**	CHED	1839	**Zhang, X.**	PMSE	242
Zhang, Q.	BIOL	28	**Zhang, W.**	CHED	2079	**Zhang, X.**	CATL	53
Zhang, Q.	CHED	111	**Zhang, W.**	COLL	442	**Zhang, X.**	CATL	499
Zhang, Q.	ENFL	373	**Zhang, W.**	ENVR	264	**Zhang, X.**	CELL	289
Zhang, Q.	ENFL	508	**Zhang, W.**	ENVR	430	**Zhang, X.**	ENFL	272
Zhang, Q.	INOR	1423	**Zhang, W.**	PROF	33	**Zhang, X.**	POLY	741
Zhang, Q.	ENVR	514	**Zhang, W.**	COLL	595	**Zhang, X.**	CATL	539
Zhang, Q.	CATL	114	**Zhang, W.**	ENFL	511	**Zhang, X.**	PMSE	483
Zhang, Q.	ENFL	85	**Zhang, W.**	ANYL	17	**Zhang, Y.**	CATL	254
Zhang, Q.	I&EC	10	**Zhang, W.**	ENVR	262	**Zhang, Y.**	ANYL	450
Zhang, Q.	COMP	355	**Zhang, W.**	ENVR	285	**Zhang, Y.**	CELL	346
Zhang, Q.	ENVR	327	**Zhang, W.**	COLL	778	**Zhang, Y.**	MEDI	152
Zhang, Q.	ANYL	196	**Zhang, W.**	ENVR	128	**Zhang, Y.**	ORGN	477
Zhang, R.	INOR	846	**Zhang, W.**	ENVR	160	**Zhang, Y.**	PHYS	170
Zhang, R.	POLY	601	**Zhang, W.**	ENVR	247	**Zhang, Y.**	PHYS	399
Zhang, R.F.	MEDI	35	**Zhang, W.**	ENVR	398	**Zhang, Y.**	MEDI	367
Zhang, R.F.	MEDI	202	**Zhang, W.**	CATL	180	**Zhang, Y.**	PMSE	55
Zhang, R.	PMSE	536	**Zhang, W.**	ENFL	187	**Zhang, Y.**	POLY	326
Zhang, R.	POLY	70	**Zhang, W.**	PMSE	544	**Zhang, Y.**	ANYL	449
Zhang, R.	COLL	606	**Zhang, X.**	COLL	9	**Zhang, Y.**	BIOT	208
Zhang, S.	CATL	308	**Zhang, X.**	COLL	307	**Zhang, Y.**	COMP	252
Zhang, S.	MEDI	49	**Zhang, X.**	ENVR	655	**Zhang, Y.**	PMSE	524
Zhang, S.	INOR	713	**Zhang, X.**	MEDI	360	**Zhang, Y.**	PMSE	525
Zhang, S.	PHYS	556	**Zhang, X.**	PROF	2	**Zhang, Y.**	COLL	169
Zhang, S.	ENVR	108	**Zhang, X.**	PHYS	588	**Zhang, Y.**	CELL	88
Zhang, S.	CATL	58	**Zhang, X.**	ORGN	195	**Zhang, Y.**	COLL	306
Zhang, S.	INOR	76	**Zhang, X.**	ENVR	338	**Zhang, Y.**	BIOT	149
Zhang, S.	COLL	436	**Zhang, X.**	CATL	545	**Zhang, Y.**	ENVR	270
Zhang, S.	COLL	439	**Zhang, X.**	ENFL	143	**Zhang, Y.**	ORGN	430
Zhang, S.	PMSE	289	**Zhang, X.**	ENFL	513	**Zhang, Y.**	ORGN	434
Zhang, S.	ENFL	50	**Zhang, X.**	ENFL	532	**Zhang, Y.**	ORGN	436
Zhang, S.	ORGN	154	**Zhang, X.**	ENFL	538	**Zhang, Y.**	ORGN	557
Zhang, S.	COLL	11	**Zhang, X.**	COMP	123	**Zhang, Y.**	ANYL	388
Zhang, S.	ENVR	718	**Zhang, X.**	MEDI	49	**Zhang, Y.**	ANYL	196
Zhang, S.	POLY	645	**Zhang, X.**	ENFL	346	**Zhang, Y.**	INOR	722
Zhang, S.	POLY	516	**Zhang, X.**	MEDI	2	**Zhang, Y.**	MEDI	6
Zhang, S.	POLY	545	**Zhang, X.**	BIOT	156	**Zhang, Y.**	ENFL	520
Zhang, S.	POLY	715	**Zhang, X.**	BIOT	261	**Zhang, Y.**	ENVR	757
Zhang, S.	CATL	378	**Zhang, X.**	PHYS	482	**Zhang, Y.**	INOR	67
Zhang, T.	ENFL	19	**Zhang, X.**	CATL	269	**Zhang, Y.**	INOR	481
Zhang, T.	CATL	371	**Zhang, X.**	CATL	525	**Zhang, Y.**	ORGN	73
Zhang, T.	ENFL	74	**Zhang, X.**	PMSE	473	**Zhang, Y.**	INOR	903
Zhang, T.	ENVR	305	**Zhang, X.**	CELL	319	**Zhang, Y.**	INOR	909
Zhang, T.	MEDI	19	**Zhang, X.**	BIOL	132	**Zhang, Y.**	CATL	545
Zhang, T.	PMSE	176	**Zhang, X.**	ORGN	384	**Zhang, Y.**	BIOL	206
Zhang, T.	POLY	615	**Zhang, X.**	ENVR	57	**Zhang, Y.**	POLY	251
Zhang, T.	COLL	731	**Zhang, X.**	ENVR	63	**Zhang, Y.**	ANYL	360
Zhang, T.	POLY	292	**Zhang, X.**	AGFD	31	**Zhang, Y.**	ANYL	362
Zhang, T.	POLY	365	**Zhang, X.**	BIOL	305	**Zhang, Y.**	ANYL	426
Zhang, T.	POLY	497	**Zhang, X.**	INOR	734	**Zhang, Y.**	CHED	1111

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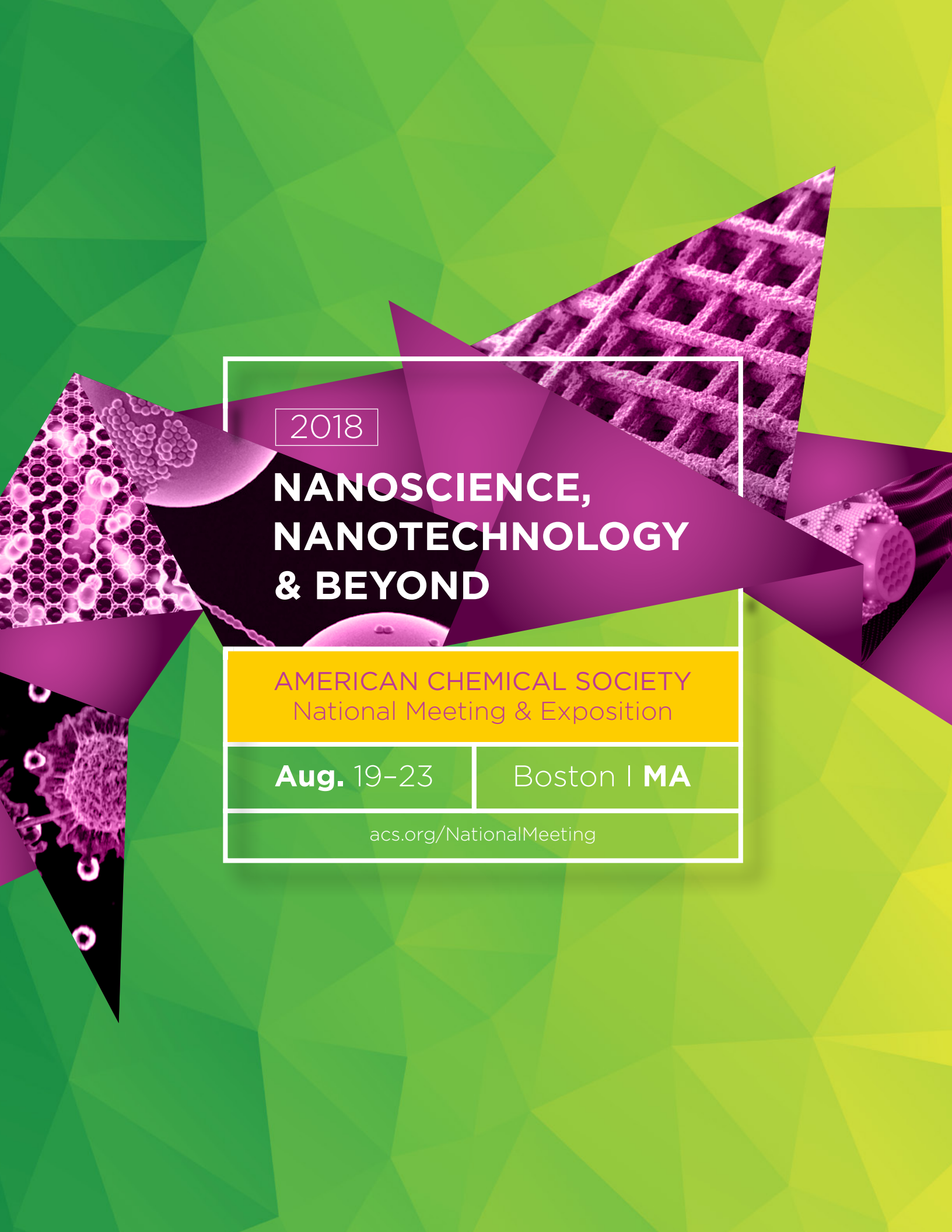

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