

**1908**  
American  
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Engineers  
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Founded



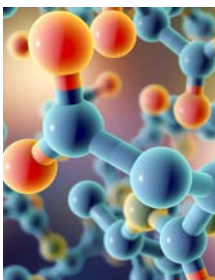
**1934**  
First Edition  
of Perry's  
*Chemical  
Engineers'  
Handbook* is  
Published



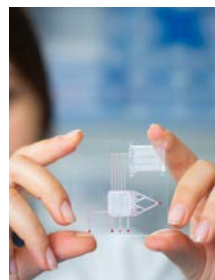
**1947**  
Fischer-Tropsch  
Process Used  
to Form  
Hydrocarbons  
from Synthetic  
Gas in the U.S.



**1958**  
General  
Electric  
Debuts Newly  
Synthesized  
Polycarbonate  
Plastics



**1970**  
Low-Loss  
Optical Fibers  
Developed  
by Corning  
Incorporated

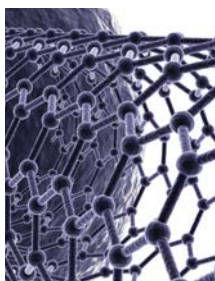


  
**18AIChE**  
Annual Meeting, Pittsburgh, PA

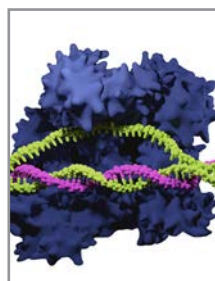
**AIChE® + Chemical Engineering:**  
**TODAY, TOMORROW & LEADING THE FUTURE**



**CONFERENCE PROGRAM • OCTOBER 28 - NOVEMBER 2 • PITTSBURGH, PA**



**1991**  
Carbon  
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(CNT) are  
Discovered by  
Sumio Iijima



**2016**  
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Using CRISPR  
Editing  
Approved by  
the NIH



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# 2018 ANNUAL MEETING CONTENTS

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To learn more about AIChE's professional development, education, and other opportunities to help you do a world of good through the Institute, just look for these icons throughout the pages of the program book:



### A Note on Sustainability at AIChE Meetings

AIChE constantly reviews the materials used at and produced for Meetings in terms of sustainability. Every attempt is made to use sustainable products within the economic framework of the meeting. Specific items may include the use of recycled or FSC certified papers, environmentally friendly inks and solvents, use of electronic (pdf) instead of printed materials, limiting the quantities produced and use of production facilities closer to the meeting site.

*Neither the American Institute of Chemical Engineers (AIChE), the presenters and author(s) of this work, their employer, nor their employer's officers and directors, warrant or represent expressly or by implication, the correctness or accuracy of the content of the information presented. As between (1) the AIChE, the presenter and author(s) of this work, their employers, and their employers' officers and directors, and (2) the user/viewer of this work, the user/viewer accepts any legal liability or responsibility whatsoever for the consequence of its use or misuse.*



A black and white photograph of two workers in hard hats and safety gear standing on a metal platform with railings. They are positioned next to a large, cylindrical industrial structure with corrugated metal siding. The structure has large text painted on it. The worker on the right is pointing towards the sky.

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# 2018 ANNUAL MEETING WELCOME



Dear Colleagues:

Welcome to Pittsburgh and our 2018 AIChE® Annual Meeting!

One hundred and ten years ago this fall, AIChE held its first Annual Meeting here in Pittsburgh. This year, we celebrate this long history of chemical engineering accomplishments while casting our collective sights on the future — where chemical engineers will play new and pivotal roles in empowering industry and improving quality-of-life.



Past, present, or future, there's plenty to celebrate this year. On Tuesday, we'll mark AIChE's anniversary at an "AIChE's 110 Years" session, where senior ChemEs and rising-stars alike will reflect on the Institute's evolution and future trajectory. Also on Tuesday, AIChE's Women's Initiatives Committee commemorates its own milestone with a 20th anniversary symposium. More than 20 prominent women ChemEs will share their research, innovations, and visions for the profession. Yet another AIChE milestone is Sunday's 20th running of the Chem-E-Car Competition®, part of the Annual Student Conference (Oct. 26–29).

This Meeting explores chemical engineering breakthroughs in new topical conferences and featured events. Supporting the efforts of AIChE's RAPID Manufacturing Institute is a topical conference devoted to Next-Gen Manufacturing — incorporating topics in process intensification, modular manufacturing, 3D printing, cybersecurity, and much more. Additional new topical conferences address societal well-being — including frontiers in immunotherapy, microbes at biomedical interfaces, and engineers' roles in food innovation.

A "Future of Energy" featured panel on Monday morning offers insight into where the energy industry is headed in the U.S. and around the globe. Speakers from the U.S. Dept. of Energy, ExxonMobil, and Abu Dhabi National Oil Company will offer valuable insights. For even more perspective, a Tuesday special session called "What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business" examines how historical disruptions have shaped the chemicals and fuels businesses, and how future disturbances could further transform those industries. Panelists will share ideas and advice on how the new generations of ChemEs can navigate the evolving industry landscape.

Supplementing all of this, the Meeting incorporates explorations of nanotechnology and nanomaterials, fossil energy R&D, green process engineering, the food-energy-water nexus, NH<sub>3</sub> energy, and sensors. Other special sessions spotlight ways to strengthen the profession through greater diversity and inclusiveness.

The Annual Meeting also shines a light on some of the profession's most distinguished people:

- On Monday morning, Sang Yup Lee (Korea Advanced Institute of Science and Technology) discusses the role of biotechnology in achieving the United Nations' sustainable development goals in his P. V. Danckwerts Lecture.
- Monday evening, AIChE's Society for Biological Engineering (SBE) sponsors the Daniel I. C. Wang Award Lecture, in which honoree John Auniņš (Seres Therapeutics) shares "Lessons from a Life in BioPharma."
- Tuesday morning's Andreas Acrivos Professional Progress Award Lecture will be delivered by Orlin Velev (North Carolina State Univ.), who will discuss microscale engineering of reconfigurable particle structures.
- Tuesday evening, SBE's James E. Bailey Award Lecture will be given by Jeffrey Hubbell (Univ. of Chicago), who will describe techniques for "Turning Immunity On and Off."
- Wednesday's John M. Prausnitz AIChE Institute Lecturer is Klavs Jensen (MIT), who will discuss methods for "Accelerating Development and Intensification of Chemical Processes."

To keep track of all these events, your first action should be to download AIChE's Annual Meeting app to your mobile device. It's the best way to manage your time and stay in-the-know. Just as important: be safe. Please read the safety information and codes of conduct included in your program book and posted by your hotel.

Finally, I hope that you will make some time to network at our Meeting's exhibit, coffee breaks, poster sessions, and receptions.

AIChE extends its sincere thanks to the Meeting's sponsors, our Meeting Program Chairs — Karl Johnson and Cliff Kowall — and our General Arrangements Chair, Susan Fullerton-Shirey. We are also grateful for the myriad presenters, authors, session chairs, and volunteers who make this Meeting possible.

I'm glad that you have joined us for this remarkable milestone Meeting. Now, on to the celebration!

Christine Seymour, PhD  
2018 AIChE President

WELCOME

A black and white photograph of a complex industrial structure, possibly an oil rig or refinery, with numerous pipes, beams, and a central vertical column. The sun is shining from the upper left, creating a bright glow and casting long shadows across the structure.

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## MEETING PROGRAM & GENERAL ARRANGEMENTS CHAIRS



### MEETING PROGRAM CHAIR

**J. Karl Johnson**

W. K. Whiteford Professor

Department of Chemical & Petroleum Engineering

Associate Director, Center for Simulation & Modeling

*University of Pittsburgh*



### MEETING PROGRAM CO-CHAIR

**Cliff Kowall**

Senior Technical Fellow – Corporate Engineer

Process Innovation & University Collaboration

*The Lubrizol Corporation (Berkshire Hathaway)*

Adjunct Faculty Member

Department of Chemical & Petroleum Engineering

*University of Pittsburgh*



### GENERAL ARRANGEMENTS CHAIR

**Susan Fullerton-Shirey**

Assistant Professor

Department of Chemical & Petroleum Engineering

*University of Pittsburgh*

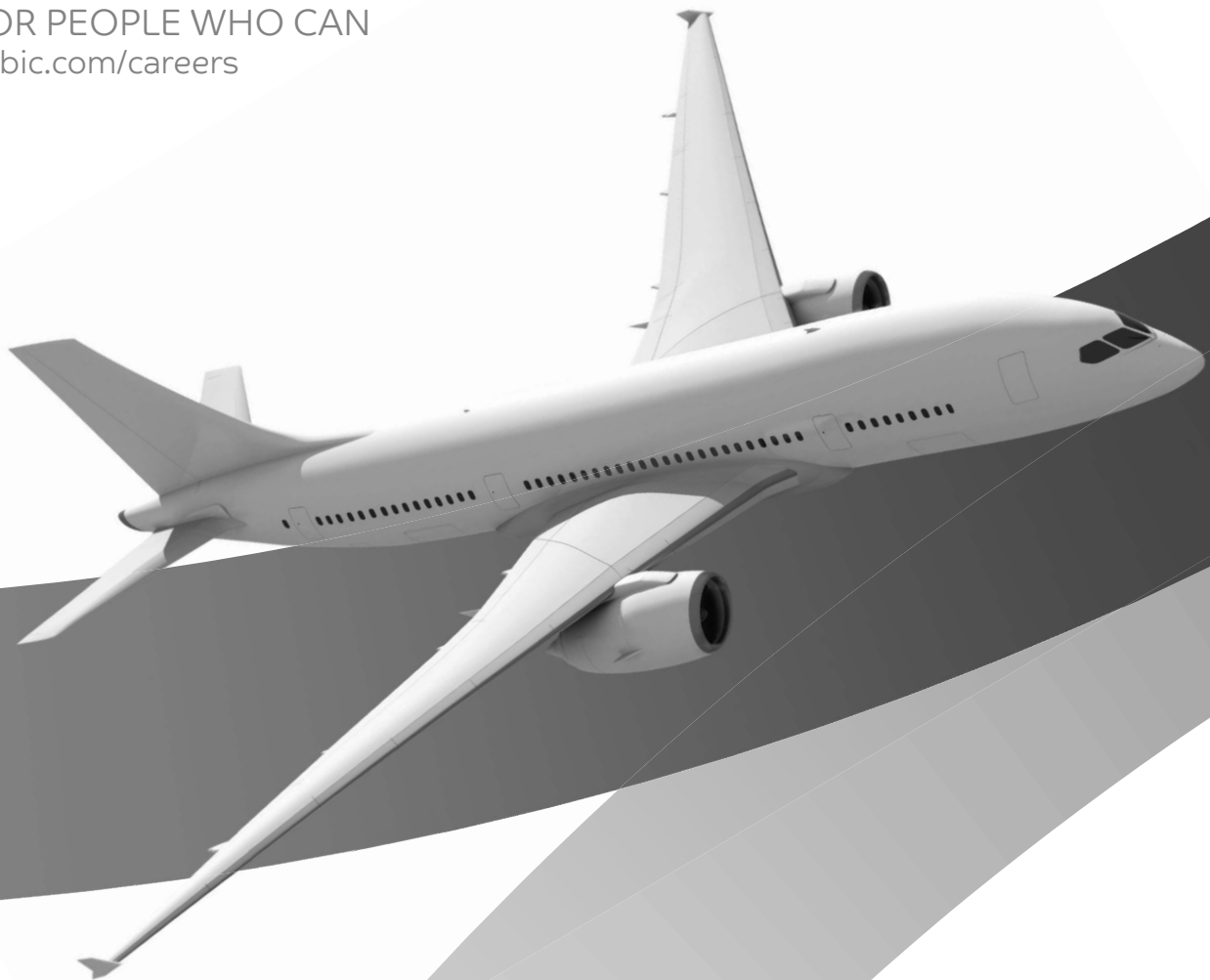
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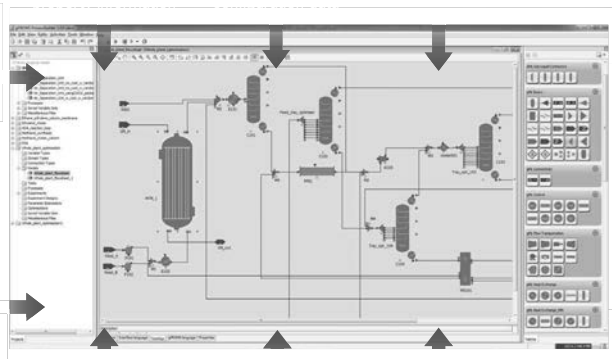
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- Alliant Insurance Services, Inc.
- American Society for Engineering Management (ASEM)
- ANSYS, Inc. \*
- AON Affinity
- AVEVA Software LLC \*
- Bruker Corporation
- Buchiglas USA Corp.
- CACHE Corp.
- Cambridge University Press
- CDS Analytical
- Chemstations
- Cognistx 
- COMSOL, Inc.
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- Equilibar
- Extrel CMS
- Flottweg Separation Technology, Inc.
- Fritsch Milling & Sizing, Inc.
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- Imperial College London
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- Innovatia \*
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- JSOL Corporation
- Knovel \*
- Malvern Panalytical
- Molecular Knowledge Systems
- Nanoscience Instruments

- National Energy Technology Laboratory 
- NIST Facility for Adsorbent Characterization & Testing 
- NOVA Chemicals
- OBG
- Optimal Industrial Technologies Ltd.
- Park Systems
- Parker Autoclave Engineers †
- Parr Instrument Company
- Powder Processing & Technology LLC
- Process Industry Practices
- Process Systems Enterprise \*
- ProSim, Inc.
- Quantachrome Instruments
- Riogen
- Rockwell Automation \*
- Royal Society of Chemistry
- SABIC
- Siemens PLM Software \* 
- Software for Chemistry & Materials
- Solvay Specialty Polymers †
- Surface Measurement Systems
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- Tech4Imaging
- Teledyne ISCO †
- Tridiagonal Solutions Inc.
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Advanced Manufacturing Processes and Research Tradeshow (AMPRT)

Exhibitors as of September 28, 2018.

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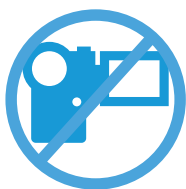


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## A NOTE ON PHOTOGRAPHY AND VIDEOGRAPHY FROM THE MEETING ORGANIZERS



AIChE Meetings are one of the primary ways the Institute fulfills its mission to advance the development and exchange of relevant knowledge.

The content presented at the AIChE Annual Meeting is the property of the presenters and the firms where they work.



**Recording of sessions or taking photos of slides is strictly prohibited.**

Thank you.

## SAFETY TIPS

Enhance your experience at the AIChE Meeting by staying safe. Here are some safety tips to observe:



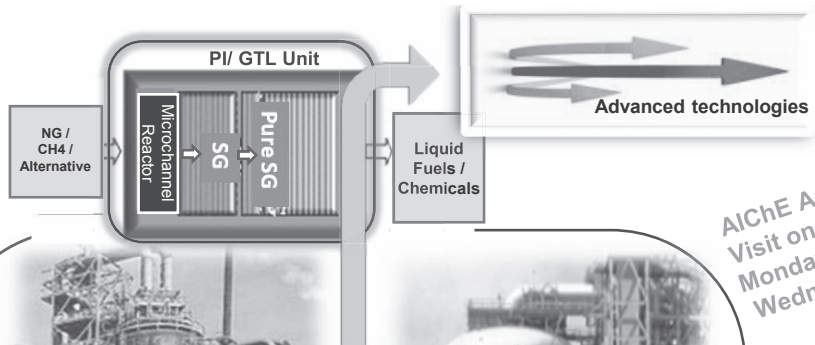
- When off the hotel grounds, please do not wear your badge in public. Doing so can give professional opportunists access to your name, which they may then exploit to your detriment.
- When you are through with your badge, turn it in to registration. Do not leave it laying in the open so that unscrupulous individuals have access to it. In addition, please do not let anyone have access to your badge for any purpose. Lending badges to others for access to the meeting is strictly prohibited.
- Have your room key out and ready when entering your hotel room. Fumbling in an attempt to locate it in either a pocket or purse outside your door could be a security risk.
- Never give a stranger your room number.
- Upon check-in to your room, note where the nearest fire exits are, so you know in which direction to go quickly in case of a fire emergency. Remember – smoke rises, so if necessary, while exiting, get as close to the floor as possible when there is heavy smoke present.
- When out in an urban area, it is advisable to travel in groups or pairs.
- Looking down and concentrating on a mobile device while texting or listening to music through earbuds can be a hazardous activity. Doing so while you are attempting to cross a street, getting on or off an escalator, walking in a crowd, or making your way through an exhibit area can all be harmful to your safety and the safety of others.

Recently, there have been many incidents of distracted meeting attendees who have attempted to walk up the down escalators or walk down the up escalators in our meeting venues.

Please take advantage of the ample seating provided in our meeting facilities in order to use your mobile device(s) in a calm setting, so that you have a safe, enjoyable experience at AIChE meetings.

- Avoid excessive consumption of alcohol. Alcohol reduces inhibitions and impairs the capacity to reason – a perfect formula to make you a target for unscrupulous behavior.

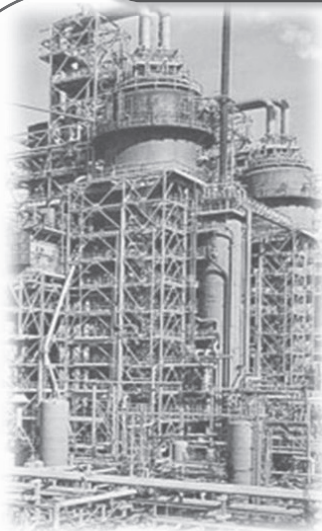
This security advisory was implemented by AIChE's Executive Board of the Program Committee (EBPC) with your safety in mind. We welcome any other suggestions you may have to help attendees have a safe and pleasant experience at our meetings.



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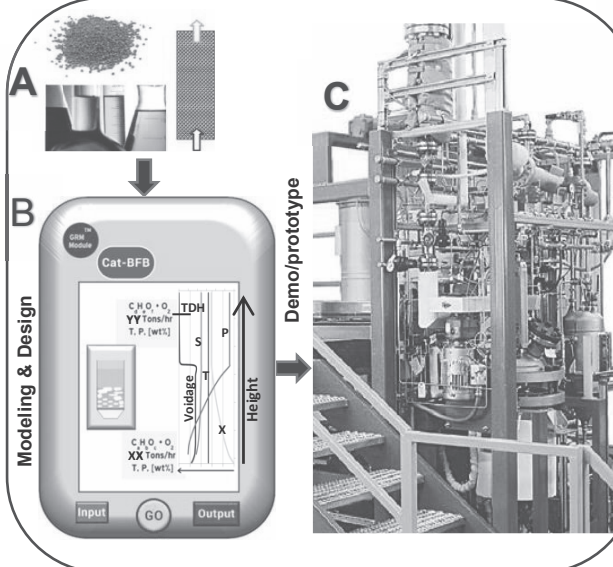
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# 2018 ANNUAL MEETING INFORMATION

## ONSITE INFORMATION AND LOGISTICS

### Onsite Registration Hours

David L. Lawrence Convention Center, Exhibit Hall B

Saturday, October 27	Noon - 5:00 PM
Sunday, October 28	8:00 AM - 8:00 PM
Monday, October 29	7:00 AM - 5:30 PM
Tuesday, October 30	7:00 AM - 5:30 PM
Wednesday, October 31	7:30 AM - 5:00 PM
Thursday, November 1	7:30 AM - 4:30 PM
Friday, November 2*	8:00 AM - 12:00 PM

\*A registration table will be available near the technical sessions taking place on Friday, November 2.

### 2018 AIChE Annual Meeting Exhibit

David L. Lawrence Convention Center, Exhibit Hall B

Sunday, October 28	1:00 PM - 3:30 PM* 6:30 PM - 7:30 PM
Monday, October 29	9:30 AM - 5:00 PM
Tuesday, October 30	9:30 AM - 5:00 PM

\*1:00pm-3:30pm on Sunday afternoon is the Meet the Faculty Candidate Poster Session. Exhibitors are not required to be present at this time, but many will be. Attendees are invited to take advantage of this opportunity to preview the exhibits while the hall is not as crowded.



### WIC Family Accommodations Room/ Mothers Room

The David L. Lawrence Convention Center has a mothers room on the 2nd floor. To get access, call 412.325.6193 (also posted on the door) and security will give you access. The room has a refrigerator and furniture.



### Recommended Daycare Services

Below is a list of daycare services recommended by Visit Pittsburgh:

Nanny Poppinz: <http://www.nannypoppinz.com>

Flexible: <http://flexablecare.com/>



### Shipping & Printing at the David L. Lawrence Convention Center

Please note that there is no business center or in-center FedEx or UPS at the David L. Lawrence Convention Center. There is a FedEx across the street from the convention center on Penn Avenue.



### Lost and Found

For questions and help with Lost and Found onsite, please go to the registration desk located in Exhibit Hall B.

## COFFEE BREAKS & REFRESHMENTS

Grab a cup of coffee and get your energy boost between technical sessions at the following events:



### Coffee Breaks

Monday, October 29 • 10:30 AM - 11:00 AM

Tuesday, October 30 • 10:30 AM - 11:00 AM

David L. Lawrence Convention Center, Exhibit Hall B



### 2018 Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture

Tuesday, October 30 • 11:15 AM - 12:15 PM

David L. Lawrence Convention Center,  
Spirit of Pittsburgh Ballroom A



### John M. Prausnitz AIChE Institute Lecture

Wednesday, October 31 • 11:15 AM - 12:15 PM

David L. Lawrence Convention Center,  
Spirit of Pittsburgh Ballroom A

## RECEPTIONS



### Annual Meeting Opening Reception

Sunday, October 28 • 6:30 PM - 7:30 PM

David L. Lawrence Convention Center, Exhibit Hall B

Enjoy cocktails and food while networking with friends and colleagues at the Annual Meeting.



### Poster Receptions

Monday through Wednesday, 3:30 PM - 5:00 PM

David L. Lawrence Convention Center, Exhibit Hall B

Dress up and join us for some Halloween fun during Wednesday's Halloween-themed poster reception!



### Concessions in Exhibit Hall B

Hungry? Take a break between sessions and grab some food at the concessions stand, located in Exhibit Hall B.

Sunday, October 28 • 11:00 AM - 3:00 PM

Monday, October 29 • 10:00 AM - 2:00 PM

Tuesday, October 30 • 10:00 AM - 2:00 PM

The menu will offer a variety of options for attendees to choose from, including salads, sandwiches, and light snacks.



Need to recharge? Charging Stations and Seating available in Exhibit Hall B.

Thank you for abiding by the AIChE Meetings Code of Conduct to foster a positive environment of trust, respect, open communications, and ethical behavior.  
[www.aiche.org/conductcode](http://www.aiche.org/conductcode)





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## DAVID L. LAWRENCE CONVENTION CENTER PITTSBURGH



# AICHE publishes a selection of journals for the chemical engineering community

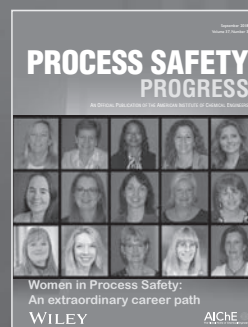
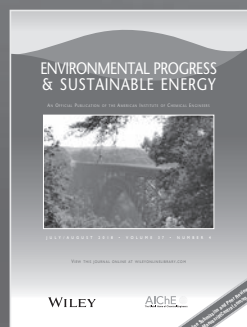
Reporting on the most exciting technological advances in core areas of chemical engineering, as well as related engineering disciplines, **AICHE Journal** is a high-impact home for quality research.

Driving impact in clinical practice and commercial healthcare products, **Bioengineering & Translational Medicine** provides rapid publication of quality research in chemical and biological engineering.

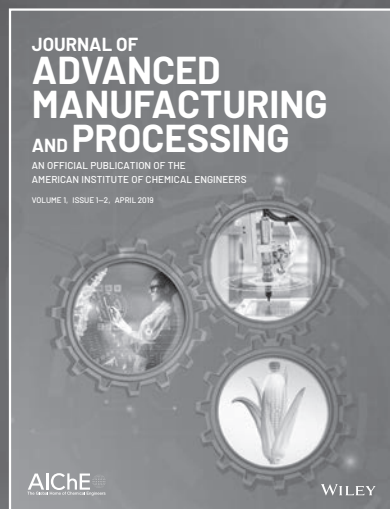
**Biotechnology Progress** focuses on research in the development and design of new processes, products, and devices for the biotechnology, biopharmaceutical and bioprocess industries.

For engineers and scientists, **Environmental Progress & Sustainable Energy** reports on critical issues of the environment, providing respected research in this important field.

With a clear focus on chemical and hydrocarbon process safety, loss prevention and health, **Process Safety Progress** is widely read by engineering professionals.



## Launching Spring 2019 *Journal of Advanced Manufacturing and Processing*



The **Journal of Advanced Manufacturing and Processing** is a peer-reviewed, online journal of the AIChE focused on capturing leading-edge, new manufacturing techniques and technologies that create and provide unique solutions to improve and enhance societal well-being.

The journal includes research articles, reviews and mini-reviews, and commentaries that apply chemical engineering principles and foundational knowledge to showcase the developments in and interdisciplinary nature of advanced manufacturing. Submissions that connect research advances to manufacturing metrics specific to the concerns they are addressing — climate, waste, and health — along with traditional economic measures are encouraged.

### Readership

Engineering professionals with specific interests in advanced manufacturing, process intensification, process enhancement, biopharmaceutical manufacturing, cell and tissue manufacturing, remanufacturing, and sustainability.

### Editorial Team

**Editor-in-Chief:** Matthew J. Realff, Georgia Institute of Technology

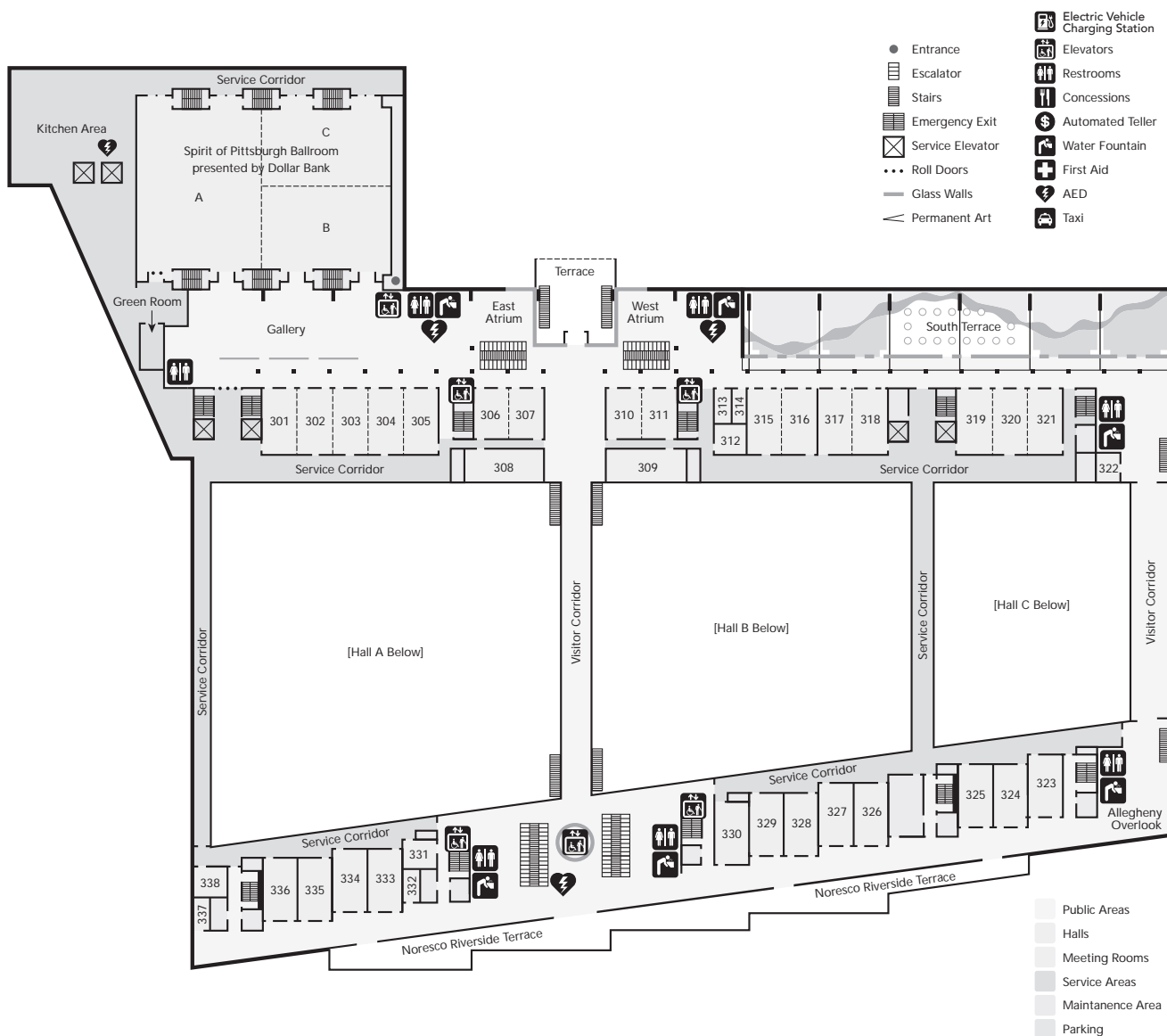
**Deputy Editor:** Jan Lerou, Jan Lerou Consulting LLC

**Deputy Editor:** Michael Rinker, Pacific Northwest National Laboratory





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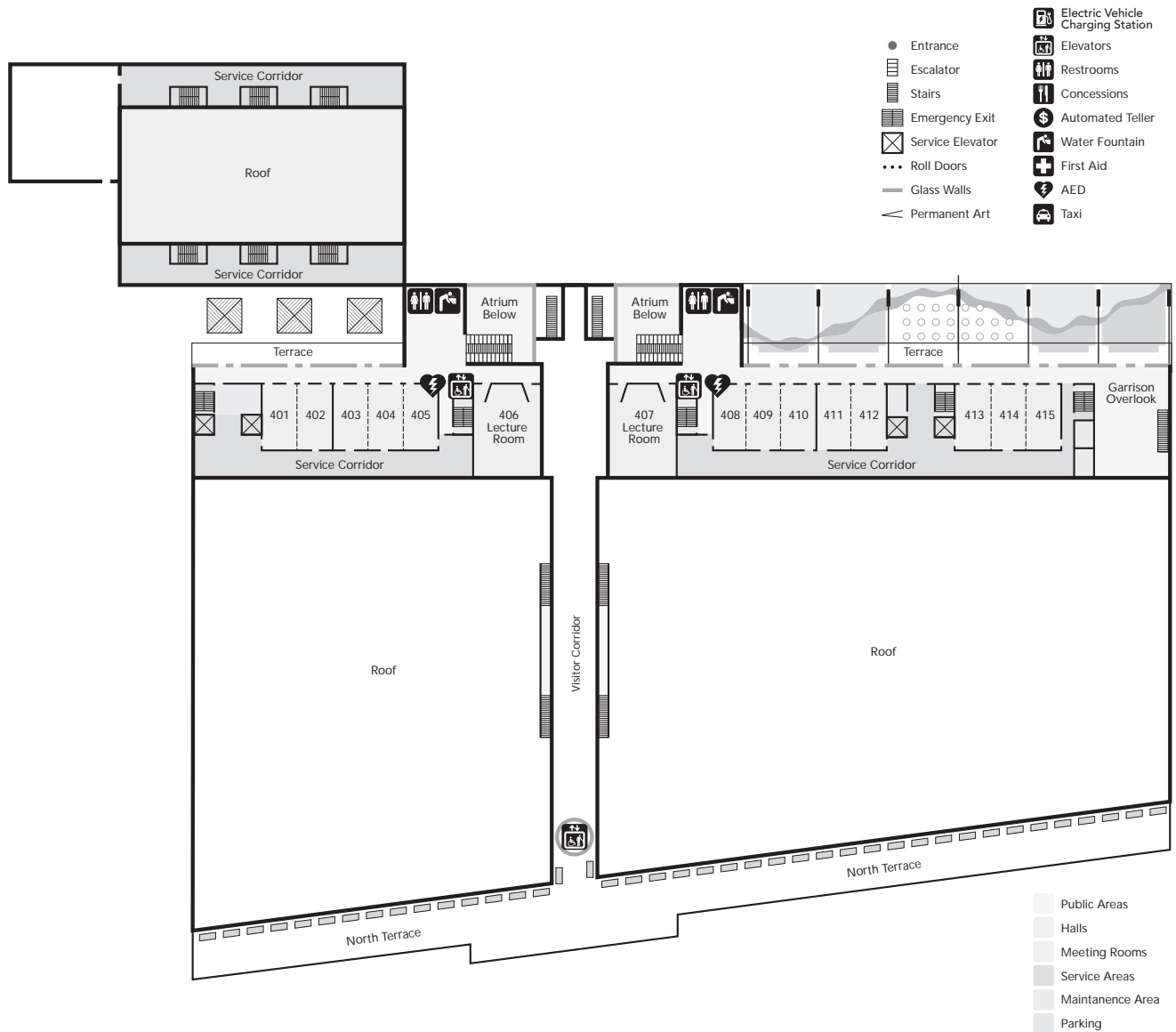
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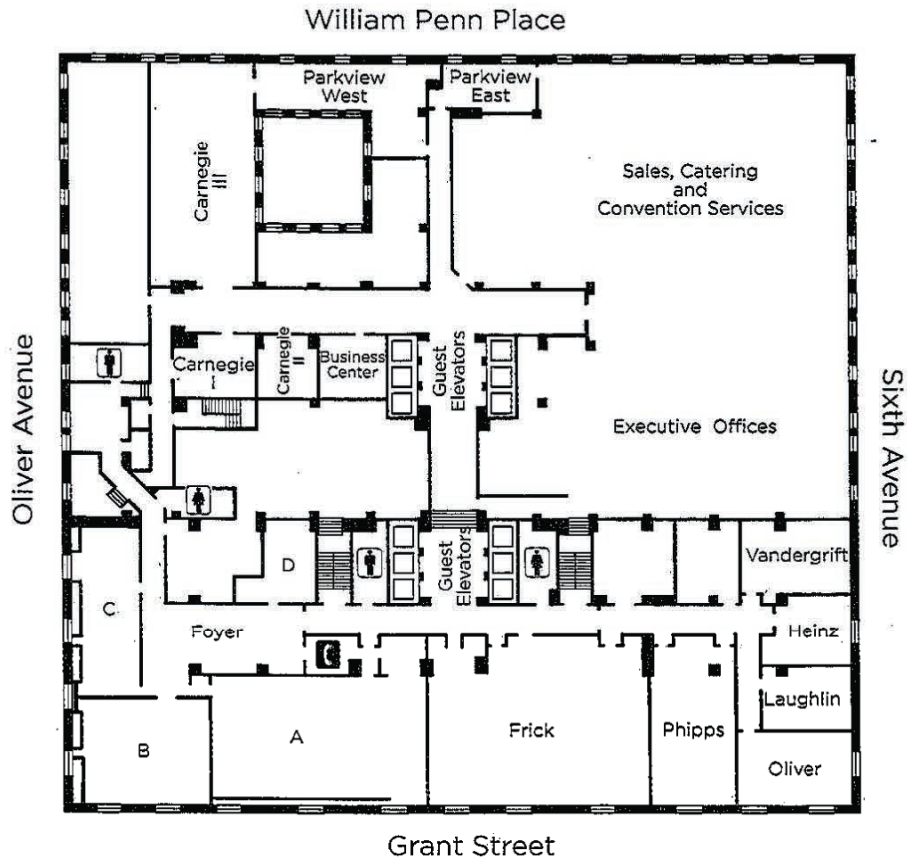
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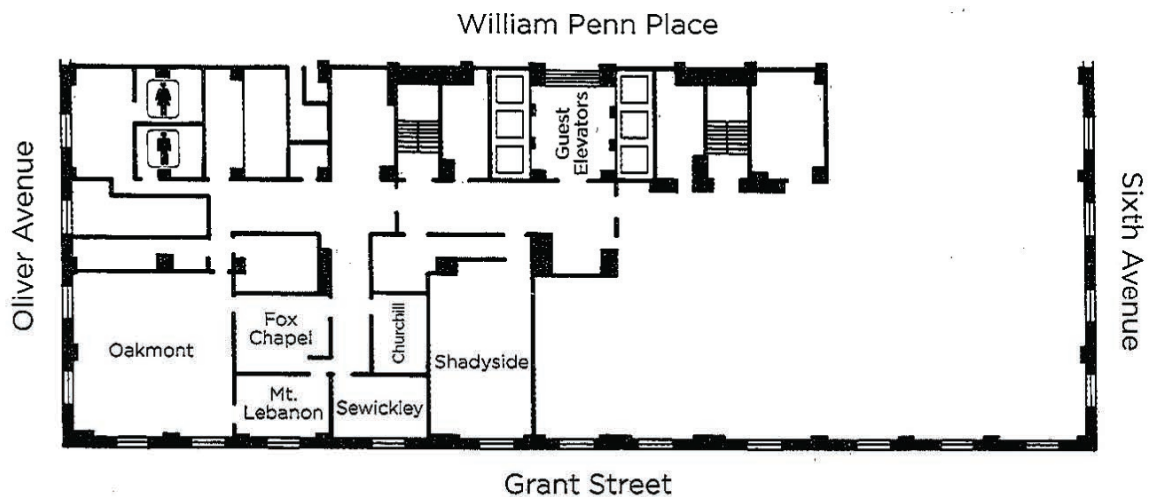


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## Conference Level



## First Floor



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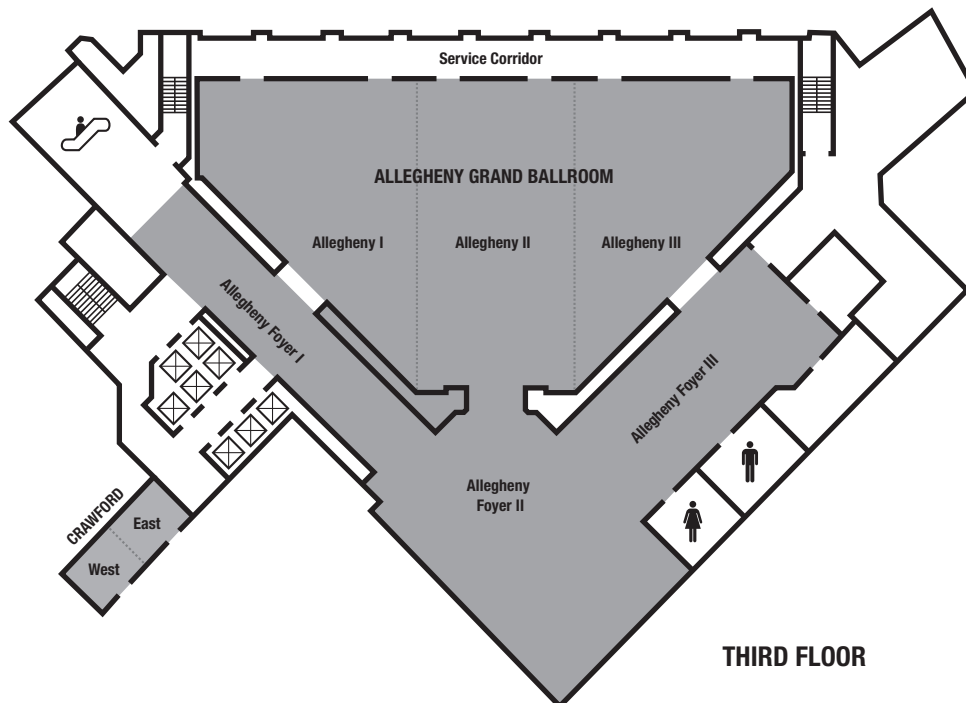
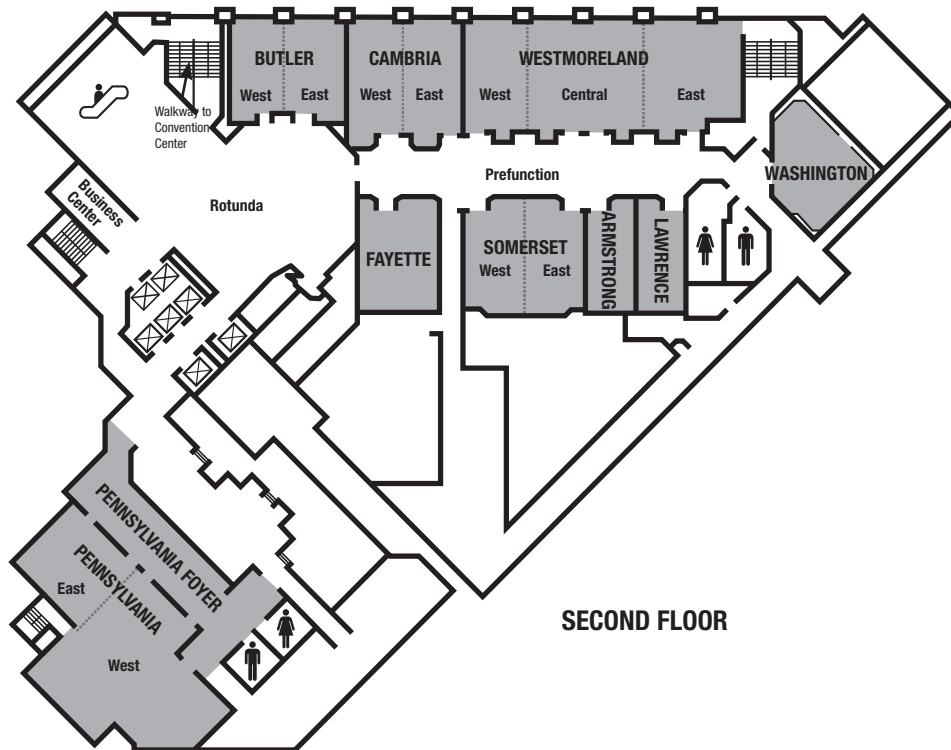
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- To engage and enrich the next generation of chemical engineers by connecting chemical engineering students with industry professionals.

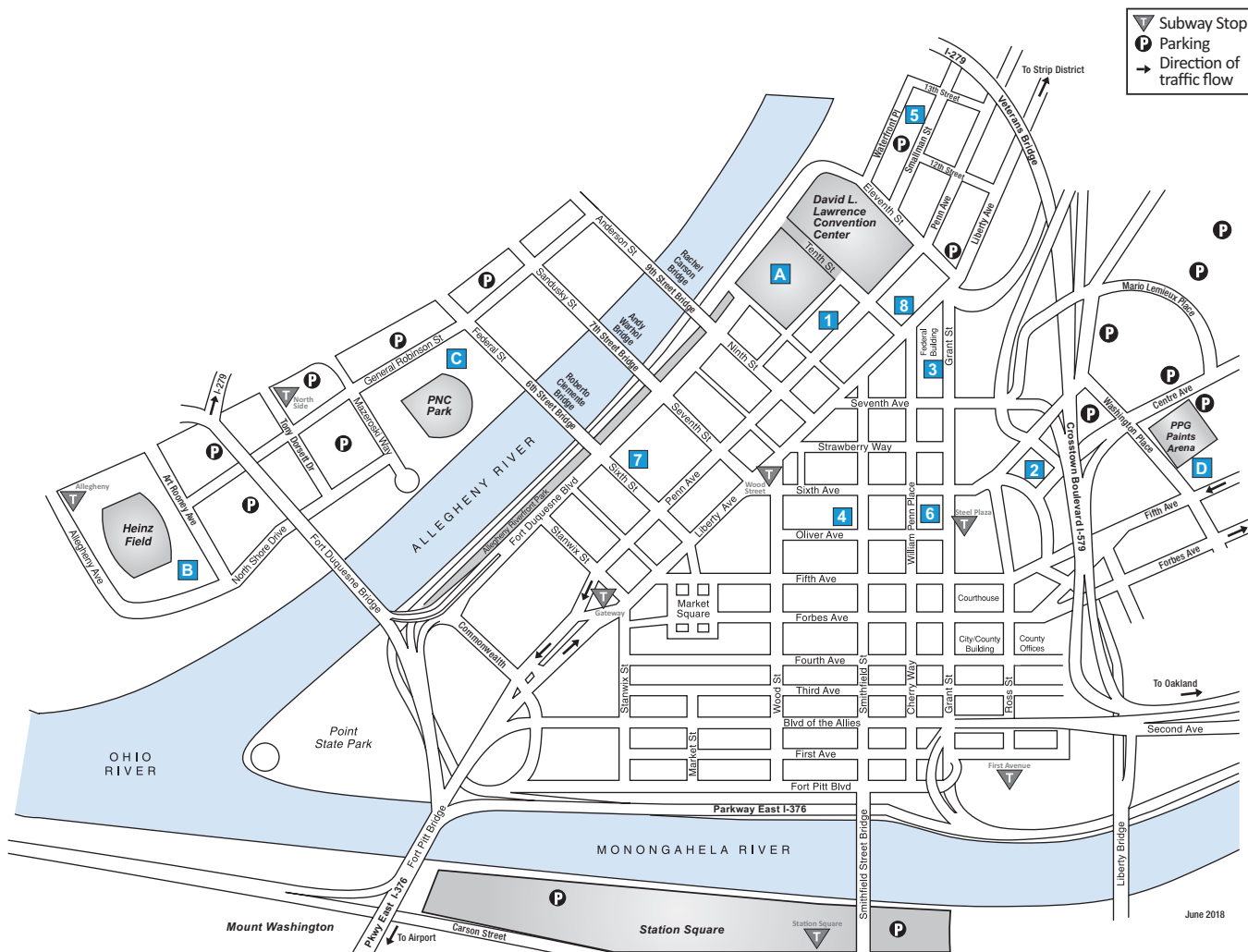
### Overview:

- ScaleUp promotes technical expertise and professionalism in the future chemical engineering workforce. Through corporate sponsorship, ScaleUp provides subsidized undergraduate membership in AIChE®, career development tools, internships and employment opportunities to chemical engineering students at 172 ABET-accredited colleges and universities in the United States and worldwide. In turn, ScaleUp corporate sponsors gain access to future engineers who are among “the best and brightest” through AIChE’s initiatives, products and networking opportunities.

### Highlights:

- Since its inception in 2007, ScaleUp has grown from 3,000 student members to over **23,000** to date.
- Since 2008, the AIChE’s Safety and Chemical Engineering Education (SChE) Certificate Program has awarded nearly **96,000** certificates to students who have demonstrated proficiency in process safety training.

To learn more about a ScaleUp corporate sponsorship, visit [www.aiche.org/scaleup](http://www.aiche.org/scaleup) or contact **Ian Sergo**, Senior Director, Business Services, AIChE at [ianse@aiche.org](mailto:ianse@aiche.org) or **646.495.1518**



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- 1 Courtyard by Marriott Pittsburgh Downtown
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- 4 Embassy Suites by Hilton Pittsburgh Downtown
- 5 Hampton Inn & Suites Pittsburgh Downtown
- 6 Omni William Penn Hotel
- 7 Renaissance Pittsburgh Hotel
- 8 Westin Convention Center Pittsburgh

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- A David L. Lawrence Convention Center
- B Heinz Field
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- D PPG Paints Arena



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# 2018 ANNUAL MEETING PROGRAM GRID KEY

The full technical program of the 2018 AIChE Annual Meeting is comprised of original programming from 22 of AIChE's divisions and forums, 10+ topical conferences, and a number of committees. Over 5,500 presentations will take place throughout the week of the Annual Meeting.

Nearly 7,000 chemical engineers working in academia and R&D will attend the premier educational forum for chemical engineers interested in innovation and professional growth. Academic and industry experts will cover a wide range of topics relevant to cutting-edge research, new technologies, and emerging growth areas in chemical engineering.

See below for a list of the subject areas covered at the 2018 AIChE Annual Meeting.

## 01 - Engineering Sciences and Fundamentals

- 01A - Thermodynamics and Transport Properties
- 01C - Interfacial Phenomena
- 01D - Transport Processes
- 01E - Electrochemical Fundamentals
- 01F - High Pressure
- 01J - Fluid Mechanics

## 02 - Separations Division

- 02A - Distillation and Absorption
- 02B - Crystallization and Evaporation
- 02C - Extractions
- 02D - Membrane-Based Separations
- 02E - Adsorption and Ion Exchange
- 02F - Fluid-Particle Separations
- 02G - Bio Separations
- 02H - General Topics and Other Methods

## 03 - Particle Technology Forum

- 03A - Particle Production and Characterization
- 03B - Fluidization and Fluid-Particle Systems
- 03C - Solids Flow, Handling and Processing
- 03D - Nanoparticles
- 03E - Energetics

## 04 - Education Division

- 04A - Undergraduate Education
- 04B - Graduate Education
- 04G - Professional Development Committee Liaison
- 04H - Career Guidance Committee Liaison
- 04I - Student Chapters Committee Liaison
- 04K - Department Heads Forum
- 04M - Young Faculty Forum

## 05 - Management Division

- 05A - Professional Development

## 06 - North American Mixing Forum

## 07 - Transport and Energy Processes Division

## 08 - Materials Engineering and Sciences Division

- 08A - Polymers
- 08B - Biomaterials
- 08D - Inorganic Materials
- 08E - Electronics and Photonics
- 08F - Composites

## 09 - Environmental Division

- 09A - Air
- 09B - Water
- 09C - Solid and Hazardous Waste
- 09D - Process Development
- 09F - Fundamentals
- 09G - Sustainability
- 09H - Climate Change

## 10 - Computing Systems and Technology Division

- 10A - Systems and Process Design
- 10B - Systems and Process Control
- 10C - Computers in Operations and Information Processing
- 10D - Applied Mathematics and Numerical Analysis
- 10E - Data and Information Systems



Please refrain from photographing slides or taking video of sessions and presentations.

# 2018 ANNUAL MEETING PROGRAM GRID KEY

## 12 - Process Development Division

- 12A - Process Research and Innovation
- 12B - Pilot Plants
- 12C - Technology Transfer and Manufacturing
- 12E - Process Intensification & Microprocess Engineering
- 12G - Product Design

## 14 - Nuclear Engineering Division

## 15 - Food, Pharmaceutical & Bioengineering Division

- 15A - Food
- 15C - Bioengineering
- 15B - Pharmaceuticals
- 15D - Engineering Fundamentals in Life Science

## 16 - Fuels and Petrochemicals Division

- 16D - Alternate Fuels and New Technology

## 17 - Forest and Plant Bioproducts Division

## 18 - Liaison Functions

- 18A - Miscellaneous
- 18B - Public Affairs and Information Committee (PAIC)
- 18C - Young Professionals Committee (YPC)
- 18D - Publication Committee
- 18E - Awards Committee
- 18G - Societal Impact Operating Council (SIOC)
- 18H - Licensing and Professional Development Committee
- 18I - Minority Affairs Committee (MAC)
- 18J - Research and New Technology Committee (RANTC)
- 18L - International Committee
- 18M - Women's Initiatives Committee (WIC)
- 18N - Assembly of Fellows
- 18O - Diversity & Inclusion

## 20 - Catalysis and Reaction Engineering Division

## 21 - Computational Molecular Science & Engineering Forum

## 22 - Nanoscale Science and Engineering Forum

- 22A - Carbon Nanomaterials
- 22B - Bionanotechnology

## 23 - Sustainable Engineering Forum

- 23A - General
- 23B - Sustainable Biorefineries
- 23C - Sustainable Energy

## 24 - Chemical Engineering & the Law Forum

## 25 - Upstream Engineering and Flow Assurance Forum

## 26 - Pharmaceutical Discovery, Development & Manufacturing Forum

## T1 - Meet the Faculty Candidate Poster Session – Sponsored by the Education Division

## T4 - 2018 International Congress on Energy (ICE)

- T4A - Biorefinery Technologies for Forest Based Lignocellulosic Biomass
- T4B - Solar Energy for Power Generation and Chemical Processing
- T4C - Hydrogen Production and Storage
- T4E - Alternative Energy & Enabling Technologies
- T4F - BioFuels
- T4G - Fossil Fuels & CCS
- T4H - International Congress on Energy (ICE) 2018

## T5 - Nanomaterials for Applications in Energy and Biology

## T6 - Next-Gen Manufacturing

- T6A - Next-Gen Manufacturing
- T6B - Process Intensification & Modular Chemical Processing
- T6C - 3D Printing

## T7 - The Food-Energy-Water Nexus

## T8 - Microbes at Biomedical Interfaces

## T9 - Sensors

## TA - Immunotherapy

## TC - Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

## TD - NH3 Energy+

## TE - Advances in Fossil Energy R&D

## TG - Innovations of Green Process Engineering for Sustainable Energy and Environment

## TJ - WIC 20th Anniversary: Celebrating Women in Chemical Engineering



An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AIChEvents app.

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# 2018 TECHNICAL PROGRAM GRID

## Property Key

DLCC = David L. Lawrence Convention Center

Omni = Omni William Penn Hotel

Westin = Westin Convention Center

## 01A - Thermodynamics and Transport Properties

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	53	Thermodynamics of Polymers*	DLCC	327
Monday	8:00 AM	74	Computational Studies of Self-Assembly	DLCC	307
Monday	8:00 AM	95	Molecular Simulation and Modeling of Complex Molecules	DLCC	309
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	159	In Honor of Pablo Debenedetti II (Invited Talks)	DLCC	307
Monday	3:30 PM	220	Faculty Candidates in CoMSEF*	DLCC	308
Monday	3:30 PM	227	In Honor of Peter Monson II (Invited Talks)	DLCC	307
Tuesday	8:00 AM	295	New Frontiers of Molecular Thermodynamics (Invited Talks)	DLCC	307
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	367	Thermophysical Properties and Phase Behavior	DLCC	307
Tuesday	3:30 PM	377	Poster Session: Thermodynamics and Transport Properties (Area 1A)	DLCC	Exhibit Hall B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	426	Thermodynamics of Biomolecular Folding and Assembly	DLCC	307
Tuesday	3:30 PM	427	Thermophysical Properties: Mixtures and Complex Systems	DLCC	305
Wednesday	8:00 AM	449	Data-Driven Screening of Chemical and Materials Space	DLCC	307
Wednesday	8:00 AM	462	Ionic Liquids: Thermodynamics and Properties*	DLCC	316
Wednesday	8:00 AM	469	Modeling of Lipid Membranes and Membrane Proteins	DLCC	309
Wednesday	12:30 PM	508	Development of Intermolecular Potential Models	DLCC	307
Wednesday	12:30 PM	527	Nucleation and Growth I*	DLCC	302
Wednesday	3:30 PM	580	Nucleation and Growth II*	DLCC	302
Wednesday	3:30 PM	587	Survey Results and Best Practices: Thermodynamics (Invited Talks)*	DLCC	405
Wednesday	3:30 PM	589	Thermodynamics at the Nanoscale	DLCC	307
Thursday	8:00 AM	614	Effects of Confinement on Molecular Properties	DLCC	307
Thursday	12:30 PM	671	Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction	DLCC	307
Thursday	3:30 PM	707	Highlights from the 20th Symposium on Thermophysical Properties (Invited Talks)	DLCC	307
Friday	8:00 AM	739	Recent Advances in Molecular Simulation Methods II*	DLCC	305
Friday	8:00 AM	741	Thermophysical Properties of Biological Systems	DLCC	307
Friday	8:00 AM	742	Thermophysical Properties: Theory and Experiments for Charged Systems	DLCC	306
Friday	12:30 PM	746	Gas Hydrates Science and Engineering	DLCC	307
Friday	12:30 PM	750	Recent Advances in Force Fields	DLCC	306

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 01C - Interfacial Phenomena

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	24	Dynamic Processes at Interfaces	Omni	Conference Center B
Sunday	3:30 PM	42	Novel Experimental Methods for the Study of Interfacial Phenomena	Omni	Frick
Sunday	3:30 PM	50	Self-Assembly in Solution	Omni	Conference Center A
Monday	8:00 AM	60	Area Plenary: Interfacial Phenomena (Invited Talks)	Omni	Conference Center A
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	166	Modeling of Interfacial Systems	Omni	Conference Center B
Monday	12:30 PM	175	Solid-Liquid Interfaces	Omni	Conference Center A
Monday	3:30 PM	192	Poster Session: Interfacial Phenomena (Area 1C)	DLCC	Exhibit Hall B
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research*	Westin	Pennsylvania East
Tuesday	8:00 AM	276	Directed and Self Assembly of Colloids	Omni	Conference Center B
Tuesday	8:00 AM	285	Fundamentals of Interfacial Phenomena I	Omni	Conference Center A
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	319	Biocolloids, Biomolecules, and Nanomaterials of Medical Relevance *	Westin	Pennsylvania East
Tuesday	12:30 PM	325	Colloidal Dispersions	Omni	Conference Center B
Tuesday	12:30 PM	342	Fundamentals of Interfacial Phenomena II	Omni	Conference Center A
Tuesday	3:30 PM	379	Active Colloidal Systems	Omni	Conference Center B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	409	Interfacial Transport Phenomena	Omni	Conference Center A
Tuesday	3:30 PM	420	Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)*	Westin	Pennsylvania East
Wednesday	8:00 AM	444	Biomolecules at Interfaces I	Omni	Conference Center B
Wednesday	8:00 AM	481	Tribute to Jacques L. Zakin: Scholar, Teacher and Mentor I (Invited Talks)	Omni	Conference Center A
Wednesday	12:30 PM	497	Biomolecules at Interfaces II	Omni	Conference Center B
Wednesday	12:30 PM	539	Tribute to Jacques L. Zakin: Scholar, Teacher and Mentor II (Invited Talks)	Omni	Conference Center A

\* This session is co-sponsored by one or more programming groups



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# 2018 TECHNICAL PROGRAM GRID

## 01C - Interfacial Phenomena

Day	Time	Session #	Session Title	Property	Room
Wednesday	3:30 PM	552	Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications	Omni	Conference Center B
Wednesday	3:30 PM	590	Tribute to Jacques L. Zakin: Scholar, Teacher and Mentor III (Invited Talks)	Omni	Conference Center A
Thursday	8:00 AM	615	Emulsions and Foams I	Omni	Conference Center A
Thursday	8:00 AM	623	Interfacial Aspects of Oil/Gas Recovery and Remediation	Omni	Conference Center B
Thursday	12:30 PM	660	Emulsions and Foams II	Omni	Conference Center A
Thursday	12:30 PM	668	Interfacial Phenomena in Electrochemical Systems	Omni	Conference Center B
Thursday	3:30 PM	709	Interfacial Phenomena in Ionic Liquids	Omni	Conference Center B
Thursday	3:30 PM	722	Soft Matter Electrokinetics	Omni	Conference Center A

## 01D - Transport Processes

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	84	Fundamental Research in Transport Processes	Omni	Conference Center B
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	3:30 PM	230	Mathematical Modeling of Transport Processes	Omni	Conference Center B
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	319	Biocolloids, Biomolecules, and Nanomaterials of Medical Relevance *	Westin	Pennsylvania East
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303

## 01E - Electrochemical Fundamentals

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	79	Electrocatalysis and Photoelectrocatalysis I: Fundamentals of CO <sub>2</sub> Reduction *	DLCC	401
Monday	8:00 AM	93	Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage*	DLCC	318
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	145	Electrocatalysis and Photoelectrocatalysis II: Reactors and Processes for CO <sub>2</sub> Reduction*	DLCC	401
Monday	3:30 PM	217	Electrocatalysis and Photoelectrocatalysis III: Hydrogen Evolution Reaction*	DLCC	401

\* This session is co-sponsored by one or more programming groups



# 2018 TECHNICAL PROGRAM GRID

## 01E - Electrochemical Fundamentals

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research*	Westin	Pennsylvania East
Tuesday	8:00 AM	279	Electroactive Biomaterials to Sense and Control Microbial Infections*	Westin	Pennsylvania East
Tuesday	8:00 AM	280	Electrocatalysis and Photoelectrocatalysis IV: Advances in Fuel Cell Catalysts*	DLCC	401
Tuesday	8:00 AM	308	Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)	DLCC	306
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	334	Electrocatalysis and Photoelectrocatalysis V: Oxygen Evolution Reaction*	DLCC	401
Tuesday	12:30 PM	335	Electrochemical Fundamentals: Faculty Candidate Session	DLCC	306
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	399	Electrocatalysis and Photoelectrocatalysis VI: Biomass Processing and Ammonia Synthesis*	DLCC	401
Tuesday	3:30 PM	400	Electrochemical Engineering: Industry-Relevant Problems and Solutions	DLCC	306
Wednesday	8:00 AM	459	Free Short Course - Redox Flow Batteries: From Fundamentals to Applications	DLCC	306
Wednesday	12:30 PM	510	Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions I	DLCC	306
Wednesday	3:30 PM	561	Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions II	DLCC	306
Thursday	8:00 AM	625	Lithium and Beyond: Fundamental Advances in High Performance Batteries I	DLCC	306
Thursday	12:30 PM	669	Lithium and Beyond: Fundamental Advances in High Performance Batteries II	DLCC	306
Thursday	3:30 PM	701	Electrochemistry for Applications in Sustainability	DLCC	306

## 01F - High Pressure

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	88	High Pressure Phase Equilibria and Modeling	DLCC	306
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	164	Materials Synthesis and Processing with Compressed or Supercritical Fluids	DLCC	306
Monday	3:30 PM	245	Thermodynamic and Transport Properties Under Pressure	DLCC	306
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Thursday	3:30 PM	721	Reactions in Near-Critical and Supercritical Fluids *	DLCC	404

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 01J - Fluid Mechanics

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	99	Novel Complex Flows (Invited Talks)	Omni	Frick
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	138	Colloidal Hydrodynamics: Structure and Microrheology	Omni	Frick
Monday	12:30 PM	155	Hydrodynamics of Active Systems	Omni	Phipps
Monday	3:30 PM	237	Poster Session: Fluid Mechanics	Omni	Frick
Tuesday	8:00 AM	268	Colloidal and Soft Matter Hydrodynamics	Omni	Frick
Tuesday	8:00 AM	307	Turbulent and Reactive Flows	Omni	Phipps
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	349	Microfluidic and Nanoscale Flows: Multiphase Systems and External Fields	Omni	Frick
Tuesday	12:30 PM	354	Particulate and Multiphase Flows: Particle and Suspension Dynamics	Omni	Phipps
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	412	Microfluidic and Nanoscale Flows: Separations & Particulates	Omni	Frick
Tuesday	3:30 PM	419	Particulate and Multiphase Flows: Theory & Experiment	Omni	Phipps
Wednesday	8:00 AM	460	Hydrodynamics of Biological Systems	Omni	Frick
Wednesday	8:00 AM	461	Interfacial and Nonlinear Flows: Particle-Laden Systems	Omni	Phipps
Wednesday	12:30 PM	503	Complex Fluids: Macromolecules	Omni	Frick
Wednesday	12:30 PM	518	Interfacial and Nonlinear Flows: Drops, Bubbles and Films	Omni	Phipps

## 02 - Separations Division

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	41	Novel Catalytic and Separation Process Based on Ionic Liquids*	DLCC	318
Monday	8:00 AM	77	Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)	DLCC	301
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	3:30 PM	227	In Honor of Peter Monson II (Invited Talks)*	DLCC	307
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	333	Division Plenary: Major Separations Challenges	DLCC	305
Tuesday	3:30 PM	376	Poster Session: Separations Division	DLCC	Exhibit Hall B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Wednesday	8:00 AM	462	Ionic Liquids: Thermodynamics and Properties*	DLCC	316
Wednesday	8:00 AM	477	Separation Processes and Waste Management*	DLCC	326

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 02A - Distillation and Absorption

Day	Time	Session #	Session Title	Property	Room
Tuesday	8:00 AM	277	Distillation Processes Fundamentals, Developments, and Applications I	DLCC	301
Tuesday	8:00 AM	300	Refining and Petrochemical Plant Modelling and Operations Improvements I*	DLCC	323
Tuesday	12:30 PM	332	Distillation Processes Fundamentals, Developments, and Applications II	DLCC	301
Tuesday	12:30 PM	362	Refining and Petrochemical Plant Modelling and Operations Improvements II*	DLCC	323

## 02B - Crystallization and Evaporation

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	207	Area 2B Plenary: In Honor of Doraiswami Ramkrishna's 80th Birthday (Invited Talks)	DLCC	302
Tuesday	8:00 AM	270	Continuous Crystallization Processes	DLCC	302
Tuesday	12:30 PM	330	Crystallization of Pharmaceutical and Biological Molecules	DLCC	302
Wednesday	8:00 AM	468	Modeling and Control of Crystallization	DLCC	302
Wednesday	12:30 PM	527	Nucleation and Growth I	DLCC	302
Wednesday	3:30 PM	580	Nucleation and Growth II	DLCC	302
Thursday	8:00 AM	610	Crystallization Process Development	DLCC	302
Thursday	12:30 PM	684	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond I	DLCC	302
Thursday	3:30 PM	723	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond II	DLCC	302
Friday	8:00 AM	737	Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions	DLCC	302

## 02C - Extractions

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	214	Developments in Extractive Separations: Processes	DLCC	303
Tuesday	8:00 AM	275	Developments in Extractive Separations: Solvents	DLCC	303
Tuesday	12:30 PM	339	Extractive Separations Fundamentals and Design	DLCC	303

## 02D - Membrane-Based Separations

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	18	Bioinspired Membranes and Membrane Processes	DLCC	302
Sunday	3:30 PM	28	Fuel Cell Membranes	DLCC	303
Sunday	3:30 PM	35	Membrane Formation	DLCC	304
Monday	3:30 PM	226	In Honor of Neal Chung I: Gas Separation	DLCC	304
Monday	3:30 PM	244	Surface Engineered and Responsive Membranes	DLCC	301
Tuesday	8:00 AM	288	In Honor of Neal Chung II: Liquid Separation	DLCC	304
Tuesday	12:30 PM	344	In Honor of Neal Chung III: Novel Membranes and Processes	DLCC	304
Tuesday	3:30 PM	396	Diffusion in Polymers*	DLCC	327
Wednesday	8:00 AM	463	Membrane-Based Organic Solvent Separations	DLCC	303

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# 2018 TECHNICAL PROGRAM GRID

## 02D - Membrane-Based Separations

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	464	Membrane Reactors	DLCC	304
Wednesday	12:30 PM	491	Advanced Polymeric Membranes for Gas Separation	DLCC	303
Wednesday	12:30 PM	516	Highly Selective Separations with Membranes I	DLCC	304
Wednesday	12:30 PM	519	Membranes for Bioseparations*	DLCC	301
Wednesday	3:30 PM	551	Advanced Inorganic Materials for Membrane Gas Separation	DLCC	303
Wednesday	3:30 PM	567	Highly Selective Separations with Membranes II	DLCC	304
Thursday	8:00 AM	609	Charged Polymers for Membrane-Based Water and Energy Applications	DLCC	305
Thursday	8:00 AM	627	Membrane Modeling and Simulation	DLCC	304
Thursday	8:00 AM	628	Membranes for CO <sub>2</sub> Capture	DLCC	303
Thursday	12:30 PM	673	Mixed-Matrix Materials for Gas Separation	DLCC	303
Thursday	12:30 PM	686	Water Treatment, Desalination, and Reuse I	DLCC	304
Thursday	3:30 PM	727	Water Treatment, Desalination, and Reuse II	DLCC	304
Friday	8:00 AM	743	Water Treatment, Desalination, and Reuse III	DLCC	304
Friday	12:30 PM	752	Water Treatment, Desalination, and Reuse IV	DLCC	304

## 02E - Adsorption and Ion Exchange

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	128	Area Plenary: Adsorption and Ion Exchange I - In Honor of Peter Monson I (Invited Talks)	DLCC	301
Monday	3:30 PM	219	Experimental Methods and Characterization of Adsorbent Materials	DLCC	311
Monday	3:30 PM	239	PSA/TSA	DLCC	305
Tuesday	8:00 AM	260	Area Plenary: Adsorption and Ion Exchange II: Fundamentals and Applications	DLCC	305
Tuesday	3:30 PM	373	Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange	DLCC	Exhibit Hall B
Wednesday	8:00 AM	436	Adsorption Applications for Sustainable Energy and Chemicals	DLCC	311
Wednesday	8:00 AM	478	Structured Adsorbents: Beyond Pellets and Beads	DLCC	305
Wednesday	12:30 PM	506	CO <sub>2</sub> Capture By Adsorption	DLCC	334
Wednesday	12:30 PM	520	Molecular Simulation of Adsorption I	DLCC	305
Wednesday	3:30 PM	550	Adsorbent Materials for Sustainable Energy and Chemicals	DLCC	301
Wednesday	3:30 PM	572	Molecular Simulation of Adsorption II	DLCC	305
Thursday	8:00 AM	594	Adsorbent Materials	DLCC	309
Thursday	8:00 AM	612	Diffusion, Transport and Dynamics in Adsorption Systems	DLCC	310
Thursday	12:30 PM	641	Adsorbent Materials: MOFs I	DLCC	305
Thursday	12:30 PM	657	Chromatographic Separations and SMB	DLCC	309
Thursday	3:30 PM	687	Adsorbent Materials: MOFs II	DLCC	305

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# 2018 TECHNICAL PROGRAM GRID

## 02F - Fluid-Particle Separations

Day	Time	Session #	Session Title	Property	Room
Thursday	8:00 AM	596	Advances in Fluid Particle Separations	DLCC	301
Thursday	12:30 PM	646	Application of Solid-Liquid Separation Technologies to Produced Water	DLCC	301
Thursday	3:30 PM	703	Fluid Particle Separation in Industrial and Environmental Systems	DLCC	301
Friday	8:00 AM	740	Solid-Fluid Separations in Oil & Gas Production and Refining Processes	DLCC	303
Friday	12:30 PM	751	Techniques for Removing Fine and Ultrafine Particles from Gaseous, Aqueous or Non-Aqueous Media	DLCC	303

## 02G - Bio Separations

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	438	Advances in Bioseparations	DLCC	301
Wednesday	12:30 PM	499	Bioseparations and Downstream Processing*	Westin	Somerset
Wednesday	12:30 PM	519	Membranes for Bioseparations	DLCC	301

## 02H - General Topics and Other Methods

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	32	Hybrid Separation Processes	DLCC	301
Tuesday	3:30 PM	374	Poster Session: General Topics on Separations	DLCC	Exhibit Hall B

## 03 - Particle Technology Forum

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I*	DLCC	333
Monday	8:00 AM	56	3D Printing II*	DLCC	333
Monday	12:30 PM	123	3D Printing Keynote (Invited Talks)*	DLCC	333
Tuesday	8:00 AM	252	Advancements in Polymers and Amorphous Solids for Pharmaceutical Process Development *	Westin	Fayette
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	336	Enabling and Advanced Formulations in Drug Product Processing I: Focus on Dissolution*	Westin	Washington
Tuesday	3:30 PM	375	Poster Session: Particle Technology Forum	DLCC	Exhibit Hall B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Wednesday	12:30 PM	529	Particle Technology Awards Lectures (Invited Talks)	DLCC	415
Thursday	8:00 AM	596	Advances in Fluid Particle Separations*	DLCC	301
Thursday	8:00 AM	610	Crystallization Process Development*	DLCC	302
Friday	8:00 AM	737	Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions*	DLCC	302

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# 2018 TECHNICAL PROGRAM GRID

## 03A - Particle Production and Characterization

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	71	Characterization, Modeling and Control/Optimization of Micro- and Nano-Structured Particulate Systems	DLCC	413
Monday	12:30 PM	170	Particle Breakage and Comminution Processes	DLCC	413
Monday	3:30 PM	205	Agglomeration and Granulation Processes	DLCC	413
Tuesday	8:00 AM	298	Particle Engineering and Design for Product Value Enhancement	DLCC	413
Tuesday	12:30 PM	358	Population Balance Modeling for Particle Formation Processes: Nucleation, Aggregation and Breakage Kernels	DLCC	414
Thursday	12:30 PM	684	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond I*	DLCC	302
Thursday	3:30 PM	723	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond II*	DLCC	302

## 03B - Fluidization and Fluid-Particle Systems

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	87	Fundamentals of Fluidization	DLCC	415
Monday	12:30 PM	150	Experimental Investigation of Fluidization Processes	DLCC	415
Monday	3:30 PM	213	Computational Modeling and Validation for Fluidization Processes	DLCC	415
Tuesday	8:00 AM	267	Circulating Fluidized Beds and Measurement Techniques	DLCC	415
Tuesday	12:30 PM	364	Special Session: Celebrating Career Accomplishments of Prof. Yutaka Tsuji (Invited Talks)	DLCC	415
Tuesday	3:30 PM	406	Industrial Application of Computational and Numerical Approaches to Particle Flow	DLCC	415
Thursday	8:00 AM	617	Fluidization in Chemical Looping Processes (Area 20B)	DLCC	415
Thursday	12:30 PM	663	Fluidization and Fluid-Particle Systems for Energy and Environmental Applications	DLCC	415

## 03C - Solids Flow, Handling and Processing

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	44	Particle Technology: Educational Efforts	DLCC	415
Monday	8:00 AM	94	Modeling of Particulate Systems	DLCC	414
Monday	12:30 PM	143	Dynamics and Modeling of Particulate Systems: Discrete and Continuum	DLCC	414
Monday	3:30 PM	224	Heat Transfer in Particulate Systems	DLCC	414
Tuesday	8:00 AM	301	Solids Handling and Processing in Particulate Systems	DLCC	414
Tuesday	3:30 PM	414	Mixing and Segregation of Particulates	DLCC	414
Wednesday	8:00 AM	480	Transport of Particulate Solids (Mechanical, Pneumatic and Hydraulic Conveying/Slurry)	DLCC	414
Thursday	8:00 AM	631	Particle Separations (Solid/Solid, Solid/Liquid, Solid/Gas)	DLCC	414
Thursday	12:30 PM	656	Characterization and Measurement in Powder Processing	DLCC	414

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FLUIDIZATION XVI

May 26-31, 2019  
Guilin, China  
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# 2018 TECHNICAL PROGRAM GRID

## 03D - Nanoparticles

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	133	Area 8E Plenary: Electronic and Photonic Materials: Industry and Academia (Invited Talks)*	DLCC	330
Tuesday	12:30 PM	340	Functional Nanoparticles	DLCC	413
Tuesday	3:30 PM	405	Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles	DLCC	413
Wednesday	8:00 AM	472	Novel Nanoparticles and Nanostructured Materials for Catalysis	DLCC	415
Wednesday	12:30 PM	538	Synthesis and Assembly of Electronic and Photonic Materials*	DLCC	330
Wednesday	3:30 PM	578	Novel Nanoparticles and Nanostructured Materials for Environmental Applications	DLCC	413
Thursday	8:00 AM	630	Novel Nanoparticles and Nanostructured Materials for Energy Applications	DLCC	413
Thursday	12:30 PM	678	Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications I	DLCC	413
Thursday	3:30 PM	714	Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications II	DLCC	413

## 03E - Energetics

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	435	Additive Manufacturing of Energetics	DLCC	413
Wednesday	12:30 PM	493	Advances in Processing and Handling of Energetic Materials	DLCC	414
Wednesday	3:30 PM	564	Energetic Materials: Engineered Particles and Interfaces I	DLCC	412
Thursday	8:00 AM	616	Energetic Materials: Engineered Particles and Interfaces II	DLCC	412

## 04 - Education

Day	Time	Session #	Session Title	Property	Room
Sunday	1:00 PM	6	Meet the Faculty Candidate Poster Session*	DLCC	Exhibit Hall B
Sunday	3:30 PM	23	Chemical Engineers for a World of Good: Bringing Hard and Soft Engineering Skills and Sustainability to Undergraduates*	DLCC	315
Monday	8:00 AM	106	Teaching with Technology	DLCC	408
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	149	Experiences in Teaching Process Safety*	DLCC	335
Monday	3:30 PM	181	Networking for Nerds: How to Create Your Dream Career*	DLCC	330
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research*	Westin	Pennsylvania East
Monday	3:30 PM	229	International House of Chemical Engineers	DLCC	410
Monday	4:45 PM	248	Marketing is Not Bragging: How to Articulate Your Value to Advance Your Career*	DLCC	330
Tuesday	8:00 AM	278	Education Division Award Winners: Service, Innovation, and Research (Invited Talks)	DLCC	411
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B

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# 2018 TECHNICAL PROGRAM GRID

## 04 - Education

Day	Time	Session #	Session Title	Property	Room
Tuesday	12:30 PM	324	Catalyzing the Unique Abilities of Students with Disabilities (Invited Talks)	DLCC	411
Tuesday	12:30 PM	345	In Honor of the 2017 Recipient of the Warren K. Lewis Award (Invited Talks)	DLCC	412
Tuesday	3:30 PM	372	Poster Session: Chemical Engineering Education	DLCC	Exhibit Hall B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Wednesday	8:00 AM	449	Data-Driven Screening of Chemical and Materials Space*	DLCC	307

## 04A - Undergraduate Education

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	55	Workshop: Effective Teaching for New or Prospective Faculty	DLCC	411
Monday	8:00 AM	78	Effective Classroom and Laboratory Demonstrations	DLCC	406
Monday	8:00 AM	82	Free Forum on Engineering Education: First Year and Sophomore Year	DLCC	411
Monday	12:30 PM	153	Free Forum on Engineering Education: Junior and Senior Years I	DLCC	411
Monday	3:30 PM	221	Free Forum on Engineering Education: Junior and Senior Years II	DLCC	411
Wednesday	8:00 AM	479	Teaching Communication Skills to Engineers (Written, Oral, Data Visualization)	DLCC	411
Wednesday	12:30 PM	489	ABET Updates and Insights (Invited Talks)	DLCC	407
Wednesday	12:30 PM	541	Workshop: Teaching Design (Products, Processes, and Industry Involvement)	DLCC	413
Wednesday	3:30 PM	587	Survey Results and Best Practices: Thermodynamics (Invited Talks)	DLCC	405

## 04B - Graduate Education

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	54	Workshop: Best Practices in Research Mentoring	DLCC	413
Wednesday	3:30 PM	565	Free Forum on Engineering Education: Graduate Students	DLCC	404

## 04G - Professional Development Committee Liaison

Day	Time	Session #	Session Title	Property	Room
Sunday	10:00 AM	4	Workshop: Career Planning for Prospective Faculty	DLCC	408
Monday	3:30 PM	225	How Summer School Improved My Teaching	DLCC	409
Tuesday	8:00 AM	291	Jumpstart Your Teaching!: Small Teaching Ideas for Course Improvement	DLCC	406

## 04H - Career Guidance Committee Liaison

Day	Time	Session #	Session Title	Property	Room
Wednesday	12:30 PM	526	NSF Workshop I: Highlights from CBET	DLCC	411
Wednesday	3:30 PM	579	NSF Workshop II: Proposal Writing and Discussions with Program Managers	DLCC	411

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## 04I - Student Chapters Committee Liaison

Day	Time	Session #	Session Title	Property	Room
Sunday	12:30 PM	5	Chem-E-Car Competition	DLCC	Exhibit Hall C
Monday	8:00 AM	97	National Student Paper Competition	DLCC	410
Monday	8:00 AM	105	Student Design Competition	DLCC	409

## 04K - Department Heads Forum

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	450	Department Heads Forum (Invited Talks)	DLCC	406

## 04M - Young Faculty Forum

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	483	Young Faculty Forum (Invited Talks)	DLCC	407

## 05 - Management Division

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	163	Managing Yourself: Reinventing Yourself for Your Next Role (Workshop)	DLCC	331
Monday	3:30 PM	211	Chemical Engineers and Policy-Making	DLCC	331
Monday	3:30 PM	246	World Cafe: Food-Energy-Water Nexus (Invited Talks and Panel Discussion)*	DLCC	317
Tuesday	8:00 AM	290	Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects	DLCC	331
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	348	Rising to the Challenge: Successful Leadership in Uncertain Times	DLCC	331
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	385	Applied Project Management Fundamentals: A Tutorial	DLCC	331
Wednesday	8:00 AM	450	Department Heads Forum (Invited Talks)*	DLCC	406

## 05A - Professional Development

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	181	Networking for Nerds: How to Create Your Dream Career*	DLCC	330

## 06 - North American Mixing Forum

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	98	Novel and Unconventional Mixers	DLCC	334
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B

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# 2018 TECHNICAL PROGRAM GRID

## 06 - North American Mixing Forum

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	165	Mixing in Rheologically Complex Fluids	DLCC	334
Tuesday	8:00 AM	297	Numerical Analyses of Mixing Processes in Bioreactors	DLCC	334
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	368	The Use of CFD and Analysis Tools in Understanding of Mixing Processes	DLCC	334
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	428	The Use of CFD in Simulation of Multiphase Mixing Processes	DLCC	334
Wednesday	8:00 AM	466	Mixing Scale-up/Scale-down Issues in Pharmaceutical and Biopharmaceuticals Processes	DLCC	334
Wednesday	3:30 PM	577	North American Mixing Forum Award Session (Invited Talks)	DLCC	334

## 07 - Transport and Energy Processes

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	49	Rechargeable / Secondary Battery Technologies for Energy Storage	DLCC	324
Monday	8:00 AM	83	Fuel Cells, Electrolyzers, and Electrochemical Devices	DLCC	324
Monday	8:00 AM	103	Redox Flow Batteries for Energy Storage	DLCC	323
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	174	Solar Energy for Power Generation and Chemical Processing I*	DLCC	324
Monday	3:30 PM	243	Solar Energy for Power Generation and Chemical Processing II*	DLCC	324
Tuesday	8:00 AM	259	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas	DLCC	324
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	329	CO <sub>2</sub> Capture, Utilization, and Disposal: Key to Clean Energy Production	DLCC	324
Tuesday	3:30 PM	378	Poster Session: Transport and Energy Processes	DLCC	Exhibit Hall B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Wednesday	8:00 AM	457	Experimental, Theoretical, and Numerical Analysis of Transport Processes in Flow Reactors	DLCC	324
Wednesday	12:30 PM	490	Advanced Fuel Cell, Hydrogen Generation & Storage Technologies	DLCC	324
Friday	8:00 AM	733	Modeling and Computation in Energy and Environment*	DLCC	310

## 08 - Materials Engineering and Sciences Division

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I*	DLCC	333
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	3:30 PM	193	Poster Session: Materials Engineering & Sciences (08A - Polymers)	DLCC	Exhibit Hall B
Monday	3:30 PM	194	Poster Session: Materials Engineering & Sciences (08B - Biomaterials)	DLCC	Exhibit Hall B
Monday	3:30 PM	195	Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)	DLCC	Exhibit Hall B

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## 08 - Materials Engineering and Sciences Division

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	196	Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)	DLCC	Exhibit Hall B
Monday	3:30 PM	197	Poster Session: Materials Engineering & Sciences (08F - Composite Materials)	DLCC	Exhibit Hall B
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Wednesday	8:00 AM	451	Division Plenary: Materials Engineering & Sciences Division (Invited Talks)	DLCC	327

## 08A - Polymers

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I*	DLCC	333
Sunday	3:30 PM	16	Biobased Intermediates and Biomaterials*	DLCC	335
Sunday	3:30 PM	45	Polymer Thin Films, Nanoconfinement, and Interfaces	DLCC	309
Sunday	3:30 PM	53	Thermodynamics of Polymers	DLCC	327
Monday	8:00 AM	59	Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering I (Invited Talks)	DLCC	327
Monday	12:30 PM	129	Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering II (Invited Talks)	DLCC	327
Monday	3:30 PM	193	Poster Session: Materials Engineering & Sciences (08A - Polymers)*	DLCC	Exhibit Hall B
Tuesday	8:00 AM	284	Excellence in Graduate Polymer Research (Invited Talks)	DLCC	327
Tuesday	12:30 PM	356	Polymers in Additive Manufacturing*	DLCC	333
Tuesday	12:30 PM	357	Polymers in Industry - Rising Stars (Invited Talks)	DLCC	327
Tuesday	3:30 PM	396	Diffusion in Polymers	DLCC	327
Tuesday	3:30 PM	417	Nanostructured Polymers and Composites	DLCC	330
Wednesday	12:30 PM	521	Multiscale and Coarse-Grained Modeling of Polymers	DLCC	326
Wednesday	12:30 PM	524	Nanoscale Phenomena in Macromolecular Systems	DLCC	327
Wednesday	12:30 PM	531	Polymer Processing and Rheology	DLCC	333
Wednesday	3:30 PM	573	Nanoscale Structure in Polymers	DLCC	327
Wednesday	3:30 PM	576	New Methods in Polymer Modeling	DLCC	326
Wednesday	3:30 PM	581	Polymer Phase Change and Assembly	DLCC	333
Wednesday	3:30 PM	582	Polymer Reaction Engineering	DLCC	324
Thursday	8:00 AM	608	Charged and Ion-Containing Polymers	DLCC	327
Thursday	8:00 AM	609	Charged Polymers for Membrane-Based Water and Energy Applications*	DLCC	305
Thursday	8:00 AM	632	Polymers in Batteries	DLCC	326
Thursday	12:30 PM	648	Atomistic and Molecular Modeling and Simulation of Polymers	DLCC	330
Thursday	12:30 PM	650	Biomacromolecular Gels	DLCC	326
Thursday	12:30 PM	670	Mechanics, Structure, and Properties in Polymers	DLCC	331
Thursday	12:30 PM	680	Polymers for Energy Storage and Conversion	DLCC	327

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## 08A - Polymers

Day	Time	Session #	Session Title	Property	Room
Thursday	3:30 PM	708	Inhomogeneous Polymers	DLCC	331
Thursday	3:30 PM	716	Polyelectrolytes and Polymer Electrolytes	DLCC	327
Thursday	3:30 PM	717	Polymer Characterization	DLCC	326
Thursday	3:30 PM	718	Polymer Networks and Gels	DLCC	330
Friday	8:00 AM	729	Bio-Based Polymers	DLCC	319
Friday	8:00 AM	731	Crosslinked Polymers	DLCC	320

## 08B - Biomaterials

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I*	DLCC	333
Sunday	3:30 PM	16	Biobased Intermediates and Biomaterials*	DLCC	335
Sunday	3:30 PM	17	Biobased Materials: Design and Application*	Westin	Westmoreland West-Central
Sunday	3:30 PM	19	Biomaterials for in vitro Tissue Models and Improved Therapeutic Strategies	DLCC	331
Sunday	3:30 PM	33	Hydrogel Biomaterials	DLCC	328
Sunday	3:30 PM	39	Nanostructured Biomimetic and Biohybrid Materials and Devices*	DLCC	311
Monday	8:00 AM	64	Biomaterials	DLCC	311
Monday	8:00 AM	65	Biomaterials and Life Science Engineering: Faculty Candidates	DLCC	328
Monday	8:00 AM	69	Cells, Organs, and Labs on a Chip I: Modeling Cell Interactions*	Westin	Cambria
Monday	12:30 PM	131	Area Plenary: Leaders in Biomaterials (Invited Talks)	DLCC	328
Monday	12:30 PM	154	Functional Interfaces to Control Pathogenic or Beneficial Microbes*	Westin	Pennsylvania East
Monday	3:30 PM	194	Poster Session: Materials Engineering & Sciences (08B - Biomaterials)*	DLCC	Exhibit Hall B
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research*	Westin	Pennsylvania East
Tuesday	8:00 AM	264	Biomaterials for Drug Delivery	DLCC	328
Tuesday	8:00 AM	279	Electroactive Biomaterials to Sense and Control Microbial Infections*	Westin	Pennsylvania East
Tuesday	8:00 AM	282	Engineering the Tissue and Cell Microenvironment I: Development and Disease*	Westin	Butler
Tuesday	12:30 PM	319	Biocolloids, Biomolecules, and Nanomaterials of Medical Relevance *	Westin	Pennsylvania East
Tuesday	12:30 PM	337	Engineering the Tissue and Cell Microenvironment II: Directing Cell Behavior with Extracellular Cues*	Westin	Butler
Tuesday	12:30 PM	353	Nucleic Acid Materials and Delivery	DLCC	328
Tuesday	3:30 PM	386	Biomaterials: Graduate Student Award Session	DLCC	328
Tuesday	3:30 PM	420	Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)*	Westin	Pennsylvania East
Wednesday	8:00 AM	452	Drug Delivery I: Biologics*	Westin	Cambria

\* This session is co-sponsored by one or more programming groups



June 23-27, 2019  
New York, NY  
<http://synbiocoference.org/2019>



# 2018 TECHNICAL PROGRAM GRID

## 08B - Biomaterials

Day	Time	Session #	Session Title	Property	Room
Wednesday	12:30 PM	496	Biomaterial Scaffolds for Tissue Engineering I: Musculoskeletal Applications	DLCC	328
Wednesday	12:30 PM	498	Bionanotechnology for Gene and Drug Delivery I*	DLCC	309
Wednesday	12:30 PM	509	Drug Delivery II: Small Molecules*	Westin	Cambria
Wednesday	3:30 PM	554	Biomaterial Scaffolds for Tissue Engineering II: Bioactive and Drug-Eluting Materials	DLCC	328
Wednesday	3:30 PM	555	Bionanotechnology for Gene and Drug Delivery II*	DLCC	309
Wednesday	3:30 PM	559	Drug Delivery III: Systems for Administration*	Westin	Cambria
Wednesday	3:30 PM	575	Nanotechnology for Biotechnology and Pharmaceuticals II*	DLCC	311
Thursday	8:00 AM	603	Biomaterials for Immunological Applications	DLCC	331
Thursday	8:00 AM	604	Biomimetic Materials	DLCC	328
Thursday	8:00 AM	636	Self-Assembled Biomaterials*	DLCC	311
Thursday	12:30 PM	652	Biomaterials in Industry and the Clinic	DLCC	328
Thursday	12:30 PM	662	Engineering in Cancer Biology and Therapy I: Signaling*	Westin	Cambria
Thursday	12:30 PM	672	Micro- and Nano-Scale Technologies in Life Sciences*	Westin	Washington
Thursday	3:30 PM	690	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries II*	DLCC	325
Thursday	3:30 PM	692	Bioprinting of Scaffolds, Tissues, and Organs	DLCC	328
Thursday	3:30 PM	702	Engineering in Cancer Biology and Therapy II: Tumor Microenvironment and Mechanics*	Westin	Cambria
Friday	8:00 AM	735	Modeling of Biomaterials	DLCC	321

## 08D - Inorganic Materials

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	10	Accelerated Discovery and Development of Inorganic Materials	DLCC	329
Monday	8:00 AM	61	Area 8D (Inorganic Materials) Graduate Student Award Session	DLCC	329
Monday	12:30 PM	177	Synthesis and Application of Inorganic Materials: Synthesis	DLCC	329
Monday	3:30 PM	195	Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)*	DLCC	Exhibit Hall B
Tuesday	8:00 AM	293	MOFs, COFs, and Porous Polymer Materials: Synthesis	DLCC	329
Tuesday	8:00 AM	296	Novel Nanostructured Catalytic Materials I*	DLCC	403
Tuesday	12:30 PM	340	Functional Nanoparticles*	DLCC	413
Tuesday	12:30 PM	352	Novel Nanostructured Catalytic Materials II*	DLCC	403
Tuesday	3:30 PM	405	Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles*	DLCC	413
Tuesday	3:30 PM	425	Synthesis and Application of Inorganic Materials: Characterization	DLCC	329
Wednesday	3:30 PM	574	Nanostructured Thin Films	DLCC	329
Thursday	8:00 AM	637	Semiconducting Quantum Dots and Nanocrystals*	DLCC	330
Thursday	8:00 AM	639	Synthesis and Application of Inorganic Materials: Application	DLCC	329
Thursday	12:30 PM	674	MOFs, COFs, and Porous Polymer Materials: Characterization and Application	DLCC	329

\* This session is co-sponsored by one or more programming groups



December 10-12, 2018  
San Diego, CA  
[www.aiche.org/crispr](http://www.aiche.org/crispr)

# 2018 TECHNICAL PROGRAM GRID

## 08E - Electronics and Photonics

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	25	Electrochemical Storage Materials and Devices	DLCC	330
Monday	12:30 PM	133	Area 8E Plenary: Electronic and Photonic Materials: Industry and Academia (Invited Talks)	DLCC	330
Monday	3:30 PM	196	Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)*	DLCC	Exhibit Hall B
Tuesday	8:00 AM	262	Area 8E Graduate Student Award Finalists (Sponsored by JVST)	DLCC	330
Tuesday	8:00 AM	279	Electroactive Biomaterials to Sense and Control Microbial Infections*	Westin	Pennsylvania East
Tuesday	12:30 PM	355	Photovoltaic Materials and Devices	DLCC	330
Wednesday	12:30 PM	538	Synthesis and Assembly of Electronic and Photonic Materials	DLCC	330
Wednesday	3:30 PM	562	Electronic and Photonic Materials Devices and Theory	DLCC	330
Wednesday	3:30 PM	574	Nanostructured Thin Films*	DLCC	329
Thursday	8:00 AM	637	Semiconducting Quantum Dots and Nanocrystals	DLCC	330

## 08F - Composites

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I*	DLCC	333
Sunday	3:30 PM	37	Multifunctional Composites	DLCC	323
Monday	8:00 AM	72	Characterization of Composites	DLCC	330
Monday	3:30 PM	197	Poster Session: Materials Engineering & Sciences (08F - Composite Materials)*	DLCC	Exhibit Hall B
Monday	3:30 PM	202	3D Printing of Composites*	DLCC	333
Tuesday	12:30 PM	326	Composites for Environmental Applications	DLCC	329
Wednesday	12:30 PM	488	2D Nanocomposites: New Composites with 2-Dimensional Nanomaterials	DLCC	329
Thursday	12:30 PM	666	Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion I*	DLCC	310
Thursday	3:30 PM	688	Advanced Structural Composites	DLCC	329
Thursday	3:30 PM	706	Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion II*	DLCC	310

## 09 - Environmental Division

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	14	Applied Environmental Catalysis*	DLCC	403
Sunday	3:30 PM	23	Chemical Engineers for a World of Good: Bringing Hard and Soft Engineering Skills and Sustainability to Undergraduates*	DLCC	315
Monday	8:00 AM	73	Combustion Kinetics and Emissions*	DLCC	402
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317

\* This session is co-sponsored by one or more programming groups



November 12-14, 2018  
Houston, TX  
[www.aiche.org/space](http://www.aiche.org/space)

# 2018 TECHNICAL PROGRAM GRID

## 09 - Environmental Division

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	100	Process Research for Improved Throughput & Efficiency, and Reduced Cost & Environmental Impact*	DLCC	335
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	148	Environmental Division Awards and Honors (Invited Talks)	DLCC	319
Monday	12:30 PM	151	FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)*	DLCC	317
Monday	3:30 PM	246	World Cafe: Food-Energy-Water Nexus (Invited Talks and Panel Discussion)*	DLCC	317
Tuesday	8:00 AM	271	Conversion of Solid Wastes to Energy and/or Product*	DLCC	319
Tuesday	8:00 AM	283	Environmental Applications of Nanotechnology and Nanomaterials*	DLCC	309
Tuesday	8:00 AM	303	Sustainable Management and Uses of Post-Consumer Materials and Waste*	DLCC	315
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	326	Composites for Environmental Applications*	DLCC	329
Tuesday	12:30 PM	338	Environmental Implications of Nanomaterials: Biological Interactions*	DLCC	309
Tuesday	12:30 PM	366	The Food-Energy-Water Nexus*	DLCC	315
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	416	Nanoparticles and Health*	DLCC	309
Wednesday	3:30 PM	545	Poster Session: Environmental Division	DLCC	Exhibit Hall B
Wednesday	4:45 PM	592	Rapid Fire Session: Environmental Division	DLCC	319
Friday	8:00 AM	733	Modeling and Computation in Energy and Environment*	DLCC	310

## 09A - Air

Day	Time	Session #	Session Title	Property	Room
Tuesday	3:30 PM	416	Nanoparticles and Health*	DLCC	309
Wednesday	8:00 AM	442	Atmospheric Chemistry and Physics I	DLCC	319
Wednesday	12:30 PM	494	Atmospheric Chemistry and Physics II	DLCC	319

## 09B - Water

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	12	Advanced Oxidation Processes	DLCC	319
Monday	3:30 PM	212	Community-Based Water Treatment Innovations	DLCC	320
Thursday	8:00 AM	595	Advanced Treatment for Water Reuse and Recycling I	DLCC	319
Thursday	12:30 PM	642	Advanced Treatment for Water Reuse and Recycling II	DLCC	319
Thursday	12:30 PM	686	Water Treatment, Desalination, and Reuse I*	DLCC	304
Thursday	3:30 PM	727	Water Treatment, Desalination, and Reuse II*	DLCC	304

\* This session is co-sponsored by one or more programming groups



December 5-7, 2018  
New Brunswick, NJ  
[www.aiche.org/sps](http://www.aiche.org/sps)

# 2018 TECHNICAL PROGRAM GRID

## 09C - Solid and Hazardous Waste

Day	Time	Session #	Session Title	Property	Room
Tuesday	12:30 PM	341	Fundamentals and Applications for Hazardous Waste Treatment	DLCC	320
Tuesday	3:30 PM	404	Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization	DLCC	320
Wednesday	8:00 AM	455	Environmental Advances in Nuclear and Hazardous Waste Treatment	DLCC	320

## 09D - Process Development

Day	Time	Session #	Session Title	Property	Room
Wednesday	12:30 PM	492	Advances in Life Cycle Optimization for Process Development	DLCC	320

## 09F - Fundamentals

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	30	Fundamentals of Food, Energy, and Water Systems	DLCC	320
Monday	8:00 AM	86	Fundamentals of Environmental Kinetics and Reaction Engineering	DLCC	320
Monday	12:30 PM	151	FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)*	DLCC	317
Thursday	3:30 PM	705	Fundamentals of Sustainability Science and Engineering	DLCC	319

## 09G - Sustainability

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317
Monday	12:30 PM	151	FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)*	DLCC	317
Tuesday	8:00 AM	302	Sustainable Fuel from Renewable Resources	DLCC	320
Thursday	8:00 AM	620	Going to a Decision Point in Sustainability Analysis	DLCC	320
Thursday	12:30 PM	685	Sustainability Metrics at the Process and Product Level	DLCC	320
Thursday	3:30 PM	698	CO <sub>2</sub> Industrial, Engineering and R&D Approaches	DLCC	320

## 09H - Climate Change

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	67	Carbon Dioxide Capture Technologies and Their Use I	DLCC	319
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317
Monday	3:30 PM	209	Carbon Dioxide Capture Technologies and Their Use II	DLCC	319

## 10 - Computing Systems and Technology Division

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	51	Software Tools and Implementations for Process Systems Engineering	DLCC	410
Monday	8:00 AM	76	Division Plenary: CAST (Invited Talks)	DLCC	407
Monday	8:00 AM	106	Teaching with Technology*	DLCC	408

\* This session is co-sponsored by one or more programming groups



# 2018 TECHNICAL PROGRAM GRID

## 10 - Computing Systems and Technology Division

Day	Time	Session #	Session Title	Property	Room
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	136	CAST Director's Student Presentation Award Finalists	DLCC	408
Tuesday	8:00 AM	272	Data Mining and Machine Learning in Molecular Sciences I*	DLCC	308
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	345	In Honor of the 2017 Recipient of the Warren K. Lewis Award (Invited Talks)*	DLCC	412
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	408	Integrated Process Engineering and Economic Analysis*	DLCC	318
Thursday	8:00 AM	611	Data Mining and Machine Learning in Molecular Sciences II*	DLCC	308

## 10A - Systems and Process Design

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	141	Data Analytics in Operational Support*	Westin	Fayette
Monday	3:30 PM	185	Interactive Session: Systems and Process Design	DLCC	Exhibit Hall B
Tuesday	8:00 AM	273	Design and Operations Under Uncertainty I	DLCC	410
Tuesday	8:00 AM	274	Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems*	DLCC	321
Tuesday	8:00 AM	304	The Energy-Water Nexus*	DLCC	317
Tuesday	12:30 PM	140	Data Analytics for Process Prediction*	Westin	Fayette
Tuesday	12:30 PM	331	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I*	DLCC	317
Tuesday	12:30 PM	343	Industrial Applications in Design and Operations*	DLCC	409
Tuesday	3:30 PM	394	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II*	DLCC	317
Tuesday	3:30 PM	408	Integrated Process Engineering and Economic Analysis*	DLCC	318
Tuesday	3:30 PM	421	Process Design: Conceptualization and Analysis of Chemical Processes I	DLCC	409
Wednesday	8:00 AM	440	Advances in Industrial Modeling & Optimization: Methodologies, Tools and Applications*	DLCC	335
Wednesday	8:00 AM	470	Multivariate Experimentation and Modeling for Pharmaceutical Products and Processes*	Westin	Fayette
Wednesday	8:00 AM	474	Process Design: Conceptualization and Analysis of Chemical Processes II	DLCC	410
Wednesday	12:30 PM	537	Sustainable Energy Generation and Utilization in System Design	DLCC	410
Wednesday	3:30 PM	583	Process Intensification through Process Systems Engineering	DLCC	409
Thursday	12:30 PM	682	Process Design: Innovation for Sustainability*	DLCC	316
Thursday	3:30 PM	700	Design and Operations Under Uncertainty II	DLCC	410
Friday	12:30 PM	747	Integrated Product and Process Design	DLCC	311

\* This session is co-sponsored by one or more programming groups



An up-to-date program is available at  
[aiche.org/annual](http://aiche.org/annual) or on the AIChEEvents app.



December 10-12, 2018  
 Matrix @ Biopolis, Singapore  
[www.aiche.org/cbio](http://www.aiche.org/cbio)

# 2018 TECHNICAL PROGRAM GRID

## 10B - Systems and Process Control

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	40	Networked, Decentralized, and Distributed Control	DLCC	408
Sunday	3:30 PM	52	Supply Chain Design and Logistics*	DLCC	409
Monday	3:30 PM	184	Interactive Session: Systems and Process Control	DLCC	Exhibit Hall B
Tuesday	8:00 AM	257	Advances in Process Control I	DLCC	408
Tuesday	8:00 AM	287	Industrial Internet of Things (IIoT) Applications and Industry 4.0 Forum*	DLCC	333
Tuesday	12:30 PM	359	Predictive Control and Optimization I	DLCC	408
Tuesday	3:30 PM	382	Advances in Process Control II	DLCC	408
Tuesday	3:30 PM	392	Cybersecurity*	DLCC	333
Wednesday	8:00 AM	456	Estimation and Control of Uncertain Systems	DLCC	408
Wednesday	8:00 AM	468	Modeling and Control of Crystallization*	DLCC	302
Wednesday	12:30 PM	530	Planning and Scheduling I*	DLCC	409
Wednesday	12:30 PM	534	Process Modeling and Control Applications	DLCC	408
Wednesday	3:30 PM	584	Process Monitoring & Fault Detection*	DLCC	410
Thursday	8:00 AM	629	Modeling, Control, and Optimization of Manufacturing Systems	DLCC	408
Thursday	12:30 PM	681	Predictive Control and Optimization II	DLCC	408
Thursday	3:30 PM	696	Computational Methods in Biological and Biomedical Systems*	DLCC	408
Thursday	3:30 PM	715	Planning and Scheduling II*	DLCC	409
Friday	8:00 AM	734	Modeling, Control, and Optimization of Energy Systems	DLCC	309
Friday	12:30 PM	748	Modeling, Estimation, and Identification	DLCC	309

## 10C - Computers in Operations and Information Processing

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	52	Supply Chain Design and Logistics	DLCC	409
Monday	3:30 PM	186	Interactive Session: Systems and Process Operations	DLCC	Exhibit Hall B
Tuesday	8:00 AM	253	Advances in Deterministic Global Optimization	DLCC	409
Tuesday	8:00 AM	273	Design and Operations Under Uncertainty I*	DLCC	410
Tuesday	12:30 PM	343	Industrial Applications in Design and Operations	DLCC	409
Tuesday	12:30 PM	359	Predictive Control and Optimization I*	DLCC	408
Wednesday	8:00 AM	441	Advances in Optimization Under Uncertainty	DLCC	409
Wednesday	12:30 PM	530	Planning and Scheduling I	DLCC	409
Thursday	8:00 AM	598	Advances in Optimization with Surrogate and Mixed-Integer Models	DLCC	409
Thursday	12:30 PM	679	Operation of Energy Systems	DLCC	410
Thursday	3:30 PM	700	Design and Operations Under Uncertainty II*	DLCC	410
Thursday	3:30 PM	715	Planning and Scheduling II	DLCC	409
Friday	12:30 PM	749	Real-Time Optimization of Operations	DLCC	310

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 10D - Applied Mathematics and Numerical Analysis

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	130	Area Plenary: Future Directions in Applied Mathematics and Numerical Analysis (Invited Talks)	DLCC	409
Monday	3:30 PM	182	Interactive Session: Applied Mathematics and Numerical Analysis	DLCC	Exhibit Hall B
Tuesday	12:30 PM	315	Advances in Computational Methods and Numerical Analysis	DLCC	410
Wednesday	3:30 PM	560	Dynamics, Reduction, and Control of Distributed Parameter Systems	DLCC	408
Thursday	12:30 PM	658	Complex and Networked Chemical and Biochemical Systems	DLCC	409
Thursday	3:30 PM	696	Computational Methods in Biological and Biomedical Systems	DLCC	408
Friday	8:00 AM	733	Modeling and Computation in Energy and Environment	DLCC	310

## 10E - Data and Information Systems

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	126	Advances in Machine Learning and Intelligent Systems	DLCC	410
Monday	3:30 PM	183	Interactive Session: Data and Information Systems	DLCC	Exhibit Hall B
Tuesday	8:00 AM	272	Data Mining and Machine Learning in Molecular Sciences I*	DLCC	308
Tuesday	8:00 AM	287	Industrial Internet of Things (IIoT) Applications and Industry 4.0 Forum*	DLCC	333
Tuesday	3:30 PM	393	Data Driven Modeling and Decision Making	DLCC	410
Wednesday	3:30 PM	584	Process Monitoring & Fault Detection	DLCC	410
Thursday	8:00 AM	601	Big Data in Chemical and Pharmaceutical Processes	DLCC	410
Thursday	8:00 AM	611	Data Mining and Machine Learning in Molecular Sciences II*	DLCC	308
Friday	8:00 AM	728	Advances in Data Analysis and Information Management	DLCC	311

## 12 - Process Development Division

Day	Time	Session #	Session Title	Property	Room
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	8:00 AM	287	Industrial Internet of Things (IIoT) Applications and Industry 4.0 Forum*	DLCC	333
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Wednesday	11:15 AM	487	John M. Prausnitz AIChE Institute Lecture*	DLCC	Spirit of Pittsburgh A
Wednesday	12:30 PM	541	Workshop: Teaching Design (Products, Processes, and Industry Involvement)*	DLCC	413
Wednesday	3:30 PM	547	Poster Session: Process Development	DLCC	Exhibit Hall B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	429	Tools for Product Design*	DLCC	319
Wednesday	11:15 AM	487	John M. Prausnitz AIChE Institute Lecture*	DLCC	Spirit of Pittsburgh B
Wednesday	12:30 PM	541	Workshop: Teaching Design (Products, Processes, & Industry Involvement)*	DLCC	413
Wednesday	3:30 PM	547	Poster Session: Process Development	DLCC	Exhibit Hall B

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 12A - Process Research and Innovation

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	16	Biobased Intermediates and Biomaterials	DLCC	335
Monday	8:00 AM	93	Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage*	DLCC	318
Monday	8:00 AM	100	Process Research for Improved Throughput & Efficiency, and Reduced Cost & Environmental Impact	DLCC	335
Monday	8:00 AM	109	Young Professional Research Projects in Industry (Invited Talks)*	DLCC	303
Tuesday	12:30 PM	368	The Use of CFD and Analysis Tools in Understanding of Mixing Processes*	DLCC	334
Tuesday	3:30 PM	390	Conceptual Process Design in Refining, Petrochemicals and Gas Processing*	DLCC	323
Wednesday	8:00 AM	440	Advances in Industrial Modeling & Optimization: Methodologies, Tools and Applications	DLCC	335
Wednesday	12:30 PM	499	Bioseparations and Downstream Processing*	Westin	Somerset
Thursday	8:00 AM	610	Crystallization Process Development*	DLCC	302

## 12B - Pilot Plants

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	75	Design, Construction, and Operation of Unit Operations Labs and Pilot Plants	DLCC	336
Monday	12:30 PM	171	Pharmaceutical Process Development and Pilot Plants	DLCC	336
Monday	3:30 PM	238	Process Scale-up Techniques	DLCC	336
Tuesday	3:30 PM	408	Integrated Process Engineering and Economic Analysis*	DLCC	318
Wednesday	8:00 AM	443	Best Practices in Pilot Plants	DLCC	336
Wednesday	8:00 AM	466	Mixing Scale-up/Scale-down Issues in Pharmaceutical and Biopharmaceuticals Processes*	DLCC	334
Wednesday	3:30 PM	547	Poster Session: Process Development*	DLCC	Exhibit Hall B

## 12C - Technology Transfer and Manufacturing

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	109	Young Professional Research Projects in Industry (Invited Talks)*	DLCC	303
Monday	3:30 PM	242	Risk Reduction in - and Implementation of - Process & Technology Development	DLCC	334
Tuesday	8:00 AM	287	Industrial Internet of Things (IIoT) Applications and Industry 4.0 Forum*	DLCC	333
Thursday	8:00 AM	629	Modeling, Control, and Optimization of Manufacturing Systems*	DLCC	408
Wednesday	3:30 PM	547	Poster Session: Process Development*	DLCC	Exhibit Hall B
Thursday	8:00 AM	629	Modeling, Control, and Optimization of Manufacturing Systems*	DLCC	408

\* This session is co-sponsored by one or more programming groups



Please refrain from photographing slides or taking video of sessions and presentations.



# 2018 TECHNICAL PROGRAM GRID

## 12E - Process Intensification & Microprocess Engineering

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	56	3D Printing II*	DLCC	333
Monday	12:30 PM	123	3D Printing Keynote (Invited Talks)*	DLCC	333
Monday	3:30 PM	236	PI Topical Conference Plenary: A Look Inside the RAPID Manufacturing Institute, Co-Hosted by RAPID and F&PD*	DLCC	335
Monday	5:50 PM	756	RAPID Manufacturing Institute Open House*	DLCC	335
Tuesday	8:00 AM	258	Advances in Process Intensification	DLCC	335
Tuesday	12:30 PM	360	Process Intensification By Enhanced Heat and Mass Transfer	DLCC	335
Tuesday	3:30 PM	422	Process Intensification By Process Integration	DLCC	335
Wednesday	12:30 PM	533	Process Intensification through the Application of Microreactors, Multiphase Reactors, and Membrane Reactors	DLCC	335

## 12G - Product Design

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I*	DLCC	333
Sunday	3:30 PM	43	Panel Discussion: Chemical Process and Product Design Careers	DLCC	326
Monday	8:00 AM	56	3D Printing II*	DLCC	333
Monday	12:30 PM	123	3D Printing Keynote (Invited Talks)*	DLCC	333
Monday	12:30 PM	149	Experiences in Teaching Process Safety	DLCC	335
Tuesday	12:30 PM	365	Sustainable and Green Product Design	DLCC	319
Tuesday	3:30 PM	429	Tools for Product Design	DLCC	319
Wednesday	12:30 PM	507	Developing Process Control Strategies for Drug Product Manufacture*	Westin	Fayette
Wednesday	3:30 PM	558	Developing Process Control Strategies for Drug Substance Manufacture*	Westin	Fayette
Thursday	3:30 PM	697	Control Strategy Development for Continuous Drug Substance and Drug Product Manufacture*	Westin	Somerset

## 14 - Nuclear Engineering Division

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	180	Wilson Award Winner (Invited Talks)	DLCC	327
Monday	4:15 PM	247	Theory, Modeling, and Simulation of Nuclear Chemical Processes I	DLCC	327
Tuesday	8:00 AM	305	Theory, Modeling, and Simulation of Nuclear Chemical Processes II	DLCC	326
Tuesday	12:30 PM	351	Molten Salt Applications for Heat Transfer and Nuclear Reactors	DLCC	326
Tuesday	3:30 PM	418	Nuclear Applications of Electrochemical Engineering	DLCC	326
Wednesday	8:00 AM	455	Environmental Advances in Nuclear and Hazardous Waste Treatment*	DLCC	320
Wednesday	8:00 AM	477	Separation Processes and Waste Management	DLCC	326

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 15 - Food, Pharmaceutical & Bioengineering Division

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317
Monday	8:00 AM	89	In Honor of Doraiswami Ramkrishna's 80th Birthday I (Invited Talks)	Westin	Somerset
Monday	8:00 AM	102	Reaction Engineering in Pharmaceuticals and Fine Chemicals*	DLCC	404
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	144	Efficient Processing of Lignin to Bioproducts and Biofuels I*	DLCC	318
Monday	12:30 PM	151	FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)*	DLCC	317
Monday	12:30 PM	157	In Honor of Doraiswami Ramkrishna's 80th Birthday II (Invited Talks)	Westin	Somerset
Monday	12:30 PM	171	Pharmaceutical Process Development and Pilot Plants*	DLCC	336
Monday	3:30 PM	216	Efficient Processing of Lignin to Bioproducts and Biofuels II*	DLCC	318
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research*	Westin	Pennsylvania East
Monday	3:30 PM	246	World Cafe: Food-Energy-Water Nexus (Invited Talks and Panel Discussion)*	DLCC	317
Tuesday	8:00 AM	254	Advances in Enzymatic Catalysis I*	DLCC	405
Tuesday	8:00 AM	299	Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries*	DLCC	404
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	316	Advances in Enzymatic Catalysis II*	DLCC	405
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	398	Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)	Westin	Allegheny Grand Ballroom II
Tuesday	3:30 PM	420	Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)*	Westin	Pennsylvania East
Thursday	12:30 PM	684	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond I*	DLCC	302
Thursday	3:30 PM	696	Computational Methods in Biological and Biomedical Systems*	DLCC	408
Thursday	3:30 PM	723	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond II*	DLCC	302

## 15A - Food

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	36	Microbiomes and Metabolomes in Food, Health, and Bioprocessing	Westin	Westmoreland East
Monday	8:00 AM	57	Advances in Functional Food Production	Westin	Westmoreland East
Monday	3:30 PM	191	Poster Session: Food and Bioprocess Engineering	DLCC	Exhibit Hall B
Tuesday	8:00 AM	255	Advances in Membrane Technologies for Food and Bioprocessing	Westin	Westmoreland East
Wednesday	8:00 AM	465	Metabolic and Process Engineering for Value-Added Products from Food Processing	Westin	Westmoreland East

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

15B - Pharmaceuticals					
Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	15	Automation and High-Throughput Technologies for Pharmaceutical Discovery and Development*	Westin	Fayette
Sunday	3:30 PM	34	Innovations in Pharmaceutical Discovery, Development, and Manufacturing*	Westin	Washington
Monday	8:00 AM	56	3D Printing II*	DLCC	333
Monday	8:00 AM	77	Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)*	DLCC	301
Monday	8:00 AM	81	Forum Plenary: Pharmaceutical Discovery, Development, and Manufacturing Forum (Invited Talks)*	Westin	Allegheny Grand Ballroom II
Monday	8:00 AM	102	Reaction Engineering in Pharmaceuticals and Fine Chemicals*	DLCC	404
Monday	12:30 PM	123	3D Printing Keynote (Invited Talks)*	DLCC	333
Monday	12:30 PM	139	Computational Solid State Pharmaceuticals*	Westin	Washington
Monday	12:30 PM	141	Data Analytics in Operational Support*	Westin	Fayette
Monday	12:30 PM	160	In Honor of the 2017 Wilhelm Award Winner I (Invited Talks)*	DLCC	406
Monday	12:30 PM	171	Pharmaceutical Process Development and Pilot Plants*	DLCC	336
Monday	12:30 PM	314	Advancements in Materials Science for Powder Handling in Pharmaceutical Process Development*	Westin	Cambria
Monday	3:30 PM	200	Poster Session: Pharmaceutical*	DLCC	Exhibit Hall B
Monday	6:30 PM	250	Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony*	Westin	Allegheny Grand Ballroom II
Tuesday	8:00 AM	254	Advances in Enzymatic Catalysis I*	DLCC	405
Tuesday	8:00 AM	281	Emerging Technologies in Pharmaceutical Research and Manufacturing*	Westin	Washington
Tuesday	8:00 AM	289	In Honor of Professor D. Ramkrishna's Contributions to Biopharmaceutical Industry (Invited Talks)*	Westin	Somerset
Tuesday	8:00 AM	299	Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries*	DLCC	404
Tuesday	12:30 PM	140	Data Analytics for Process Prediction*	Westin	Fayette
Tuesday	12:30 PM	316	Advances in Enzymatic Catalysis II*	DLCC	405
Tuesday	12:30 PM	328	Continuous Processing Technologies Applied in Drug Substance Manufacturing I*	Westin	Somerset
Tuesday	12:30 PM	330	Crystallization of Pharmaceutical and Biological Molecules*	DLCC	302
Tuesday	3:30 PM	381	Advancements in Particle Engineering for Crystallization in Pharmaceutical Process Development*	Westin	Fayette
Tuesday	3:30 PM	391	Continuous Processing Technologies Applied in Drug Substance Manufacturing II*	Westin	Somerset
Tuesday	3:30 PM	398	Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)*	Westin	Allegheny Grand Ballroom II
Tuesday	3:30 PM	402	Enabling and Advanced Formulations in Drug Product Processing II: Focus on Stability*	Westin	Washington
Wednesday	8:00 AM	466	Mixing Scale-up/Scale-down Issues in Pharmaceutical and Biopharmaceuticals Processes*	DLCC	334

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 15B - Pharmaceuticals

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	470	Multivariate Experimentation and Modeling for Pharmaceutical Products and Processes*	Westin	Fayette
Wednesday	8:00 AM	473	Panel: Pharmaceutical Engineering Challenges As Approached By Chemical Engineers Outside of Pharma (Invited Talks)*	Westin	Somerset
Wednesday	12:30 PM	505	Continuous Processing Technologies Applied in Drug Product Development I*	Westin	Washington
Wednesday	3:30 PM	557	Continuous Processing Technologies Applied in Drug Product Development II*	Westin	Washington
Thursday	8:00 AM	621	Innovations in Process Analytical Technology (PAT) and In Situ Analysis*	Westin	Somerset
Thursday	8:00 AM	626	Mechanistic Models for Integrated Pharmaceutical Product and Process Design*	Westin	Fayette
Thursday	12:30 PM	645	Application of Process Modelling to Pharmaceutical Process Design and Scale-up*	Westin	Fayette
Thursday	12:30 PM	667	Innovative Technologies to Accelerate and Enhance Drug Discovery, Development, and Manufacturing*	Westin	Somerset
Thursday	12:30 PM	678	Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications I*	DLCC	413
Thursday	12:30 PM	684	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond I*	DLCC	302
Thursday	3:30 PM	714	Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications II*	DLCC	413
Thursday	3:30 PM	719	Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals*	Westin	Fayette
Thursday	3:30 PM	723	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond II*	DLCC	302

## 15C - Bioengineering

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	17	Biobased Materials: Design and Application	Westin	Westmoreland West-Central
Monday	8:00 AM	63	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion	Westin	Westmoreland West-Central
Monday	8:00 AM	68	Cell Culture Engineering & Process Design	Westin	Fayette
Monday	12:30 PM	127	Advances in Protein Expression, Post-Translational Modification and Biomanufacturing	Westin	Westmoreland East
Monday	12:30 PM	134	Biosensors, Bidiagnosis and Bioprocess Monitoring: Materials and Devices	Westin	Westmoreland West-Central
Monday	12:30 PM	154	Functional Interfaces to Control Pathogenic or Beneficial Microbes*	Westin	Pennsylvania East
Monday	3:30 PM	188	Poster Session: Bioengineering	DLCC	Exhibit Hall B
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research*	Westin	Pennsylvania East
Tuesday	8:00 AM	256	Advances in Metabolic Engineering: Biosynthetic Pathway Engineering and Enzymatic Conversion	Westin	Westmoreland West-Central

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January 6-9, 2019  
Newport Beach, CA  
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# 2018 TECHNICAL PROGRAM GRID

15C - Bioengineering					
Day	Time	Session #	Session Title	Property	Room
Tuesday	8:00 AM	265	Biosensors, Bidiagnosis and Bioprocess Monitoring: Cell and Protein Detection	Westin	Cambria
Tuesday	12:30 PM	317	Advances in Metabolic Engineering: Emerging Tools and Technologies	Westin	Westmoreland West-Central
Tuesday	12:30 PM	319	Biocolloids, Biomolecules, and Nanomaterials of Medical Relevance *	Westin	Pennsylvania East
Tuesday	12:30 PM	361	Protein Structure, Function, and Stability	Westin	Westmoreland East
Tuesday	3:30 PM	420	Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)*	Westin	Pennsylvania East
Wednesday	8:00 AM	437	Advances in Biocatalysis and Biosynthesis	Westin	Westmoreland West-Central
Wednesday	12:30 PM	499	Bioseparations and Downstream Processing	Westin	Somerset
Wednesday	12:30 PM	502	Combinatorial Techniques in Protein Engineering	Westin	Westmoreland East
Wednesday	12:30 PM	513	Emerging Tools and Enabling Technologies in Synthetic Biology: Sensors and Actuators	Westin	Westmoreland West-Central
Wednesday	3:30 PM	563	Emerging Tools and Enabling Technologies in Synthetic Biology: Design of Complex Circuits	Westin	Westmoreland West-Central
Wednesday	3:30 PM	568	Integrative Systems Biology	Westin	Butler
Wednesday	3:30 PM	585	Protein Engineering for Therapeutics	Westin	Westmoreland East
Thursday	8:00 AM	597	Advances in Metabolic Engineering of Non-Model Organisms	Westin	Westmoreland East
Thursday	8:00 AM	619	Gene Regulation Engineering: Design Principles and Tool Development	Westin	Westmoreland West-Central
Thursday	8:00 AM	634	Rational and Computational Techniques for Protein Engineering	Westin	Butler
Thursday	12:30 PM	643	Advances in Metabolic Engineering of Autotrophic Organisms	Westin	Westmoreland East
Thursday	12:30 PM	665	Gene Regulation Engineering: Medical and Biotechnological Tools and Applications	Westin	Westmoreland West-Central
Thursday	3:30 PM	711	Modeling and Engineering Cellular Communities	Westin	Westmoreland East
Thursday	3:30 PM	725	Synthetic Biology Applications	Westin	Westmoreland West-Central

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November 29 - December 1, 2018  
Clearwater, FL  
[www.aiche.org/plantsynbio](http://www.aiche.org/plantsynbio)



# 2018 TECHNICAL PROGRAM GRID

## 15D - Engineering Fundamentals in Life Science

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	19	Biomaterials for in vitro Tissue Models and Improved Therapeutic Strategies*	DLCC	331
Sunday	3:30 PM	26	Engineering in Development and Aging	Westin	Butler
Monday	8:00 AM	65	Biomaterials and Life Science Engineering: Faculty Candidates*	DLCC	328
Monday	8:00 AM	69	Cells, Organs, and Labs on a Chip I: Modeling Cell Interactions	Westin	Cambria
Monday	8:00 AM	104	Stem Cell and Tissue Engineering I: Engineering Cells	Westin	Butler
Monday	12:30 PM	176	Stem Cell and Tissue Engineering II: Engineering Tissue	Westin	Butler
Monday	3:30 PM	190	Poster Session: Engineering Fundamentals in Life Science	DLCC	Exhibit Hall B
Tuesday	8:00 AM	264	Biomaterials for Drug Delivery*	DLCC	328
Tuesday	8:00 AM	282	Engineering the Tissue and Cell Microenvironment I: Development and Disease	Westin	Butler
Tuesday	12:30 PM	320	Biomolecular Engineering	Westin	Cambria
Tuesday	12:30 PM	337	Engineering the Tissue and Cell Microenvironment II: Directing Cell Behavior with Extracellular Cues	Westin	Butler
Tuesday	12:30 PM	353	Nucleic Acid Materials and Delivery*	DLCC	328
Wednesday	8:00 AM	447	Cell Biomechanics, Adhesion and Migration I: Implications in Cancer	Westin	Butler
Wednesday	8:00 AM	452	Drug Delivery I: Biologics	Westin	Cambria
Wednesday	12:30 PM	496	Biomaterial Scaffolds for Tissue Engineering I: Musculoskeletal Applications*	DLCC	328
Wednesday	12:30 PM	509	Drug Delivery II: Small Molecules	Westin	Cambria
Wednesday	12:30 PM	528	Omics and High-Throughput Technologies	Westin	Butler
Wednesday	3:30 PM	554	Biomaterial Scaffolds for Tissue Engineering II: Bioactive and Drug-Eluting Materials*	DLCC	328
Wednesday	3:30 PM	556	Cells, Organs, and Labs on a Chip II: Tissues and Diseases	Westin	Somerset
Wednesday	3:30 PM	559	Drug Delivery III: Systems for Administration	Westin	Cambria
Thursday	8:00 AM	600	Applications in Immunology and Immunotherapy	Westin	Washington
Thursday	8:00 AM	603	Biomaterials for Immunological Applications*	DLCC	331
Thursday	8:00 AM	607	Cell Biomechanics, Adhesion and Migration II: Cell Movement	Westin	Cambria
Thursday	12:30 PM	652	Biomaterials in Industry and the Clinic*	DLCC	328
Thursday	12:30 PM	662	Engineering in Cancer Biology and Therapy I: Signaling	Westin	Cambria
Thursday	12:30 PM	672	Micro- and Nano-Scale Technologies in Life Sciences	Westin	Washington
Thursday	12:30 PM	675	Multiscale Systems Biology	Westin	Butler
Thursday	3:30 PM	692	Bioprinting of Scaffolds, Tissues, and Organs*	DLCC	328
Thursday	3:30 PM	702	Engineering in Cancer Biology and Therapy II: Tumor Microenvironment and Mechanics	Westin	Cambria
Thursday	3:30 PM	720	Quantitative Approaches to Disease Mechanisms and Therapies	Westin	Butler

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6<sup>th</sup> International Conference  
on Stem Cell Engineering

December 5-7, 2018  
Los Angeles, CA  
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# 2018 TECHNICAL PROGRAM GRID

## 16 - Fuels and Petrochemicals Division

Day	Time	Session #	Session Title	Property	Room
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	142	Developments in Petroleum and Biofuels Refining Technologies	DLCC	323
Monday	3:30 PM	236	PI Topical Conference Plenary: A Look Inside the RAPID Manufacturing Institute, Co-Hosted by RAPID and F&PD*	DLCC	335
Tuesday	8:00 AM	300	Refining and Petrochemical Plant Modelling and Operations Improvements I	DLCC	323
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	362	Refining and Petrochemical Plant Modelling and Operations Improvements II	DLCC	323
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	390	Conceptual Process Design in Refining, Petrochemicals and Gas Processing	DLCC	323
Wednesday	3:30 PM	546	Poster Session: Fuels and Petrochemicals Division	DLCC	Exhibit Hall B

## 16D - Alternate Fuels and New Technology

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	215	Developments in Unconventionals: Shale Gas, LNG, CNG, and LPG	DLCC	323
Wednesday	8:00 AM	453	Electrochemical Reactors, Fuel Cells, and Electrolyzers I	DLCC	323
Wednesday	12:30 PM	511	Electrochemical Reactors, Fuel Cells, and Electrolyzers II	DLCC	323
Thursday	8:00 AM	599	Alternative Fuels and Enabling Technologies I	DLCC	323
Thursday	12:30 PM	644	Alternative Fuels and Enabling Technology II	DLCC	323
Thursday	3:30 PM	693	Catalytic Biomass Conversion to Chemicals	DLCC	323

## 17 - Forest and Plant Bioproducts Division

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	20	Bioplastics, Biocomposites and Value-Added Uses of Biofuel Coproducts for Sustainable Manufacturing	DLCC	325
Monday	8:00 AM	70	Cellulose-Based Materials I	DLCC	325
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	137	Cellulose Based Materials II	DLCC	325
Monday	12:30 PM	144	Efficient Processing of Lignin to Bioproducts and Biofuels I*	DLCC	318
Monday	3:30 PM	199	Poster Session: Novel Products from Forest and Plant Biomass	DLCC	Exhibit Hall B
Monday	3:30 PM	216	Efficient Processing of Lignin to Bioproducts and Biofuels II*	DLCC	318
Tuesday	8:00 AM	266	Chemical Modifications and Processing of Biomaterials	DLCC	325
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	347	Lignin for Sustainable Industrial Uses	DLCC	325

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# 2018 TECHNICAL PROGRAM GRID

## 17 - Forest and Plant Bioproducts Division

Day	Time	Session #	Session Title	Property	Room
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	411	Lignocellulosic Materials	DLCC	325
Tuesday	3:30 PM	424	Separation Processes in Biorefineries*	DLCC	324
Wednesday	8:00 AM	482	USA-China Progress in Biomass Conversion Technologies I*	DLCC	325
Wednesday	12:30 PM	540	USA-China Progress in Biomass Conversion Technology II*	DLCC	325
Wednesday	3:30 PM	591	USA-China Progress in Biomass Conversion Technology III*	DLCC	325
Thursday	8:00 AM	635	Recalcitrance of Woody Biomass*	DLCC	324
Thursday	8:00 AM	640	Thermochemical Conversion of Biomass*	DLCC	325
Thursday	12:30 PM	649	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries I*	DLCC	325
Thursday	12:30 PM	651	Biomass Characterization, Pretreatment, and Fractionation I*	DLCC	324
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols*	DLCC	405
Thursday	3:30 PM	690	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries II*	DLCC	325
Thursday	3:30 PM	691	Biomass Characterization, Pretreatment, and Fractionation II*	DLCC	324
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin*	DLCC	405
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry*	DLCC	315
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks*	DLCC	315

## 18A - Miscellaneous

Day	Time	Session #	Session Title	Property	Room
Sunday	2:30 PM	7	Entrepreneurship & Investing in Early-Stage Chemical Companies	Westin	Cambria
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)	DLCC	Spirit of Pittsburgh B
Monday	3:30 PM	208	Brewing Education and Training	DLCC	329
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)	DLCC	Spirit of Pittsburgh B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)	DLCC	303

## 18B - Public Affairs and Information Committee (PAIC)

Day	Time	Session #	Session Title	Property	Room
Sunday	3:00 PM	8	Public Affairs and AIChE: A PAIC Town Hall	DLCC	307

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# 2018 TECHNICAL PROGRAM GRID

## 18C - Young Professionals Committee (YPC)

Day	Time	Session #	Session Title	Property	Room
Sunday	10:00 AM	4	Workshop: Career Planning for Prospective Faculty*	DLCC	408
Sunday	3:30 PM	43	Panel Discussion: Chemical Process and Product Design Careers*	DLCC	326
Sunday	3:30 PM	55	Workshop: Effective Teaching for New or Prospective Faculty*	DLCC	411
Sunday	4:15 PM	22	Chemical Engineering in Sustainability (YCOST) and Policy (WISE) Award Recipient Talks (Invited Talks)	DLCC	307
Monday	8:00 AM	66	Biotechnology & Materials U.G. Research Session (Invited Talks)	DLCC	302
Monday	8:00 AM	75	Design, Construction, and Operation of Unit Operations Labs and Pilot Plants*	DLCC	336
Monday	8:00 AM	109	Young Professional Research Projects in Industry (Invited Talks)	DLCC	303
Monday	12:30 PM	124	Advanced Problem Solving in the Chemical Industry I	DLCC	407
Monday	12:30 PM	146	Energy & the Environment U.G. Research Session (Invited Talks)	DLCC	302
Monday	12:30 PM	149	Experiences in Teaching Process Safety*	DLCC	335
Monday	12:30 PM	163	Managing Yourself: Reinventing Yourself for Your Next Role (Workshop)*	DLCC	331
Monday	3:30 PM	181	Networking for Nerds: How to Create Your Dream Career*	DLCC	330
Monday	3:30 PM	203	Advanced Problem Solving in the Chemical Industry II	DLCC	407
Monday	3:30 PM	223	Green Chemistry and Engineering*	DLCC	309
Monday	4:45 PM	248	Marketing is Not Bragging: How to Articulate Your Value to Advance Your Career*	DLCC	330
Tuesday	8:00 AM	251	Advanced Problem Solving in the Chemical Industry III	DLCC	407
Tuesday	8:00 AM	290	Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects*	DLCC	331
Tuesday	8:00 AM	308	Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)*	DLCC	306
Tuesday	12:30 PM	313	Advanced Problem Solving in the Chemical Industry IV	DLCC	407
Tuesday	12:30 PM	348	Rising to the Challenge: Successful Leadership in Uncertain Times*	DLCC	331
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	385	Applied Project Management Fundamentals: A Tutorial*	DLCC	331
Wednesday	8:00 AM	483	Young Faculty Forum (Invited Talks)*	DLCC	407

## 18D - Publication Committee

Day	Time	Session #	Session Title	Property	Room
Monday	1:30 PM	179	Getting Your Research Published (Invited Talks)	DLCC	303
Monday	3:30 PM	181	Networking for Nerds: How to Create Your Dream Career	DLCC	330
Monday	4:45 PM	248	Marketing is Not Bragging: How to Articulate Your Value to Advance Your Career	DLCC	330
Tuesday	3:30 PM	383	AIChE Journal Futures: New Directions in Chemical Engineering Research (Invited Talks)	DLCC	304

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# 2018 TECHNICAL PROGRAM GRID

## 18E - Awards Committee

Day	Time	Session #	Session Title	Property	Room
Monday	11:15 AM	121	2018 Danckwerts Lecture	Westin	Allegheny Grand Ballroom II
Monday	6:00 PM	249	D.I.C. Wang Award Lecture	Westin	Allegheny Grand Ballroom I
Tuesday	11:15 AM	312	Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture	DLCC	Spirit of Pittsburgh A
Tuesday	6:00 PM	433	SBE's James E. Bailey Award Lecture	Westin	Allegheny Grand Ballroom I
Wednesday	11:15 AM	487	John M. Prausnitz AIChE Institute Lecture	DLCC	Spirit of Pittsburgh A

## 18G - Societal Impact Operating Council (SIOC)

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	753	Unconscious Bias*	DLCC	304

## 18H - Licensing and Professional Development Committee

Day	Time	Session #	Session Title	Property	Room
Sunday	5:00 PM	765	Order of the Engineer	DLCC	306

## 18I - Minority Affairs Committee (MAC)

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	753	Unconscious Bias*	DLCC	304
Monday	5:30 PM	760	MAC Eminent Engineers Awards Ceremony	DLCC	325
Tuesday	11:00 AM	310	MAC/MFF Real Talk: Navigating the Academic Career Path to Tenure (Ticketed Event)	Westin	Crawford West
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303

## 18J - Research and New Technology Committee (RANTC)

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	109	Young Professional Research Projects in Industry (Invited Talks)*	DLCC	303
Thursday	2:30 PM	761	Workshop on Identifying the Gaps and Opportunities in Graduate Education to Improve Sustainability of the US Chemical Industries*	DLCC	318

## 18L - International Committee

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	229	International House of Chemical Engineers*	DLCC	410
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Wednesday	12:30 PM	512	Emerging Junior Investigator Open Innovation Forum (Invited Talks)	DLCC	331
Wednesday	3:30 PM	569	KIChE-US Chapter Open Forum (Invited Talks)	DLCC	331

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# 2018 TECHNICAL PROGRAM GRID

## 18M - Women's Initiatives Committee (WIC)

Day	Time	Session #	Session Title	Property	Room
Sunday	9:00 AM	2	Women Undergraduates Workshop (Ticketed Event)	DLCC	315
Sunday	9:00 AM	3	Developing Your Career for Women Graduate Students and Beyond (Ticketed Event)	DLCC	316
Monday	8:00 AM	753	Unconscious Bias*	DLCC	304
Monday	11:00 AM	122	WIC Luncheon (Ticketed Event)	DLCC	Spirit of Pittsburgh A
Tuesday	8:00 AM	309	WIC 20th Anniversary: Celebrating Women in Chemical Engineering I (Invited Talks)*	DLCC	Spirit of Pittsburgh A
Tuesday	12:30 PM	371	WIC 20th Anniversary: Celebrating Women in Chemical Engineering II (Invited Talks)*	DLCC	Spirit of Pittsburgh A
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	432	WIC 20th Anniversary: Celebrating Women in Chemical Engineering III (Invited Talks)*	DLCC	Spirit of Pittsburgh A

## 18N - Assembly of Fellows

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	23	Chemical Engineers for a World of Good: Bringing Hard and Soft Engineering Skills and Sustainability to Undergraduates*	DLCC	315
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B

## 18O - Diversity & Inclusion

Day	Time	Session #	Session Title	Property	Room
Sunday	9:00 AM	2	Women Undergraduates Workshop (Ticketed Event)*	DLCC	315
Sunday	9:00 AM	3	Developing Your Career for Women Graduate Students and Beyond (Ticketed Event)*	DLCC	316
Sunday	3:00 PM	8	Public Affairs and AIChE: A PAIC Town Hall*	DLCC	307
Monday	8:00 AM	753	Unconscious Bias	DLCC	304
Monday	11:00 AM	122	WIC Luncheon (Ticketed Event)*	DLCC	Spirit of Pittsburgh A
Monday	5:30 PM	760	MAC Eminent Engineers Awards Ceremony*	DLCC	325
Tuesday	8:00 AM	309	WIC 20th Anniversary: Celebrating Women in Chemical Engineering I (Invited Talks)*	DLCC	Spirit of Pittsburgh A
Tuesday	11:00 AM	310	MAC/MFF Real Talk: Navigating the Academic Career Path to Tenure (Ticketed Event)*	Westin	Crawford West
Tuesday	12:30 PM	324	Catalyzing the Unique Abilities of Students with Disabilities (Invited Talks)*	DLCC	411
Tuesday	12:30 PM	371	WIC 20th Anniversary: Celebrating Women in Chemical Engineering II (Invited Talks)*	DLCC	Spirit of Pittsburgh A

\* This session is co-sponsored by one or more programming groups



2018 AIChE Annual Gala  
December 11, 2018  
New York, NY  
[www.aiche.org/gala](http://www.aiche.org/gala)

# 2018 TECHNICAL PROGRAM GRID

## 180 - Diversity & Inclusion

Day	Time	Session #	Session Title	Property	Room
Tuesday	3:30 PM	410	LGBTQ+ Inclusion in Engineering	DLCC	Spirit of Pittsburgh B
Tuesday	3:30 PM	432	WIC 20th Anniversary: Celebrating Women in Chemical Engineering III (Invited Talks)*	DLCC	Spirit of Pittsburgh A

## 20 - Catalysis and Reaction Engineering Division

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	14	Applied Environmental Catalysis	DLCC	403
Sunday	3:30 PM	21	Catalytic Hydrogen Generation	DLCC	405
Sunday	3:30 PM	31	Green Chemical Reaction Engineering for Sustainability	DLCC	401
Sunday	3:30 PM	41	Novel Catalytic and Separation Process Based on Ionic Liquids*	DLCC	318
Sunday	3:30 PM	46	Reaction Engineering for Combustion and Pyrolysis	DLCC	402
Sunday	3:30 PM	47	Reaction Path Analysis	DLCC	404
Sunday	3:30 PM	48	Reactor Engineering for Biomass Feedstocks*	DLCC	317
Monday	8:00 AM	73	Combustion Kinetics and Emissions	DLCC	402
Monday	8:00 AM	79	Electrocatalysis and Photoelectrocatalysis I: Fundamentals of CO <sub>2</sub> Reduction	DLCC	401
Monday	8:00 AM	90	In Honor of Michael Smith's 60th Birthday I (Invited Talks)	DLCC	405
Monday	8:00 AM	101	Rational Catalyst Design I	DLCC	403
Monday	8:00 AM	102	Reaction Engineering in Pharmaceuticals and Fine Chemicals	DLCC	404
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	145	Electrocatalysis and Photoelectrocatalysis II: Reactors and Processes for CO <sub>2</sub> Reduction	DLCC	401
Monday	12:30 PM	158	In Honor of Michael Smith's 60th Birthday II (Invited Talks)	DLCC	405
Monday	12:30 PM	160	In Honor of the 2017 Wilhelm Award Winner I (Invited Talks)	DLCC	406
Monday	12:30 PM	169	New Developments in Computational Catalysis I	DLCC	402
Monday	12:30 PM	172	Rational Catalyst Design II	DLCC	403
Monday	12:30 PM	173	Reaction Chemistry and Engineering I	DLCC	404
Monday	3:30 PM	206	Alternative Fuels	DLCC	405
Monday	3:30 PM	210	Chemical and Catalytic Conversions and Processes for Renewable Feedstocks*	DLCC	316
Monday	3:30 PM	217	Electrocatalysis and Photoelectrocatalysis III: Hydrogen Evolution Reaction	DLCC	401
Monday	3:30 PM	228	In Honor of the 2017 Wilhelm Award Winner II (Invited Talks)	DLCC	406
Monday	3:30 PM	234	New Developments in Computational Catalysis II	DLCC	402
Monday	3:30 PM	240	Rational Catalyst Design III	DLCC	403
Monday	3:30 PM	241	Reaction Chemistry and Engineering II	DLCC	404
Tuesday	8:00 AM	254	Advances in Enzymatic Catalysis I	DLCC	405
Tuesday	8:00 AM	269	Computational Catalysis I: Fundamentals	DLCC	402
Tuesday	8:00 AM	280	Electrocatalysis and Photoelectrocatalysis IV: Advances in Fuel Cell Catalysts	DLCC	401

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 20 - Catalysis and Reaction Engineering Division

Day	Time	Session #	Session Title	Property	Room
Tuesday	8:00 AM	296	Novel Nanostructured Catalytic Materials I	DLCC	403
Tuesday	8:00 AM	299	Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries	DLCC	404
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	316	Advances in Enzymatic Catalysis II	DLCC	405
Tuesday	12:30 PM	322	Breakthroughs in C1 to Chemicals and Processing Engineering*	DLCC	318
Tuesday	12:30 PM	327	Computational Catalysis II: Metal and Alloy Catalysis	DLCC	402
Tuesday	12:30 PM	334	Electrocatalysis and Photoelectrocatalysis V: Oxygen Evolution Reaction	DLCC	401
Tuesday	12:30 PM	350	Microreaction Engineering I	DLCC	404
Tuesday	12:30 PM	352	Novel Nanostructured Catalytic Materials II	DLCC	403
Tuesday	12:30 PM	369	Tutorial on the Catalyst Cost Estimation Tool: Economic Insight for Catalyst Synthesis and Scale-up Research I (Invited Talks)	DLCC	406
Tuesday	3:30 PM	380	Advanced Nanomaterial Catalysts for Clean, Sustainable Technologies	DLCC	403
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	389	Computational Catalysis III: Electrocatalysis	DLCC	402
Tuesday	3:30 PM	399	Electrocatalysis and Photoelectrocatalysis VI: Biomass Processing and Ammonia Synthesis	DLCC	401
Tuesday	3:30 PM	407	In Honor of the 2018 CRE Young Investigator Award Winner (Invited Talks)	DLCC	405
Tuesday	3:30 PM	413	Microreaction Engineering II	DLCC	404
Tuesday	3:30 PM	431	Tutorial on the Catalyst Cost Estimation Tool: Economic Insight for Catalyst Synthesis and Scale-up Research II (Invited Talks)	DLCC	406
Wednesday	8:00 AM	445	Catalysis for C1 Chemistry I: Methanol Formation and Upgrading	DLCC	403
Wednesday	8:00 AM	446	Catalysis with Microporous and Mesoporous Materials I: Design and Synthesis of Materials	DLCC	404
Wednesday	8:00 AM	448	Computational Catalysis IV: Biomass Chemistry and Chemicals Production	DLCC	402
Wednesday	8:00 AM	464	Membrane Reactors*	DLCC	304
Wednesday	8:00 AM	467	Modeling and Analysis of Chemical Reactors	DLCC	405
Wednesday	8:00 AM	472	Novel Nanoparticles and Nanostructured Materials for Catalysis*	DLCC	415
Wednesday	8:00 AM	475	Reaction Engineering for Biomass Conversion I	DLCC	401
Wednesday	12:30 PM	500	Catalysis for C1 Chemistry II: Methane Reforming and Oxidation	DLCC	403
Wednesday	12:30 PM	501	Catalysis with Microporous and Mesoporous Materials II: Site Specific and Mechanistic Characterization	DLCC	404
Wednesday	12:30 PM	504	Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, and Supported Catalysts	DLCC	402
Wednesday	12:30 PM	510	Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions I*	DLCC	306
Wednesday	12:30 PM	522	Multi-Scale Modeling	DLCC	405
Wednesday	12:30 PM	535	Reaction Engineering for Biomass Conversion II	DLCC	401
Wednesday	3:30 PM	544	Poster Session: Catalysis and Reaction Engineering (CRE) Division	DLCC	Exhibit Hall B

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 20 - Catalysis and Reaction Engineering Division

Day	Time	Session #	Session Title	Property	Room
Wednesday	3:30 PM	561	Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions II*	DLCC	306
Wednesday	3:30 PM	582	Polymer Reaction Engineering*	DLCC	324
Thursday	8:00 AM	605	Catalysis for C1 Chemistry III: Methane and CO <sub>2</sub>	DLCC	403
Thursday	8:00 AM	606	Catalysis with Microporous and Mesoporous Materials III: Fundamental Catalysis and Structure-Property Relations	DLCC	404
Thursday	8:00 AM	618	Fundamentals of Catalysis I: Oxides	DLCC	401
Thursday	8:00 AM	622	In Situ and Operando Spectroscopy	DLCC	406
Thursday	8:00 AM	624	Liquid Phase Reaction Engineering	DLCC	405
Thursday	8:00 AM	638	Syngas Production and Gas-to-Liquids Technology	DLCC	402
Thursday	12:30 PM	647	Atomically Dispersed Supported Metal Catalysts I	DLCC	406
Thursday	12:30 PM	653	Catalysis with Microporous and Mesoporous Materials IV: Conversion of Renewables, Natural Gas, and Petroleum	DLCC	404
Thursday	12:30 PM	654	Catalytic Hydrocarbon Processing I: Oxidative Upgrading of Light Hydrocarbons	DLCC	403
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols	DLCC	405
Thursday	12:30 PM	659	Data Science in Catalysis I	DLCC	402
Thursday	12:30 PM	664	Fundamentals of Catalysis II: Hydrogenation in Supported Catalysis	DLCC	401
Thursday	3:30 PM	689	Atomically Dispersed Supported Metal Catalysts II	DLCC	406
Thursday	3:30 PM	691	Biomass Characterization, Pretreatment, and Fractionation II*	DLCC	324
Thursday	3:30 PM	694	Catalytic Hydrocarbon Processing II: Non-Oxidative Upgrading of Light Hydrocarbons	DLCC	403
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin	DLCC	405
Thursday	3:30 PM	699	Data Science in Catalysis II	DLCC	402
Thursday	3:30 PM	704	Fundamentals of Catalysis III: Oxidation in Supported Catalysis	DLCC	401
Thursday	3:30 PM	721	Reactions in Near-Critical and Supercritical Fluids	DLCC	404
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry	DLCC	315
Friday	8:00 AM	732	Fundamentals of Catalysis IV: Surface Reactivity	DLCC	318
Friday	8:00 AM	736	Multiphase Reaction Engineering	DLCC	316
Friday	8:00 AM	738	Pyrolysis of Biomass	DLCC	317
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks	DLCC	315
Friday	12:30 PM	745	Fundamentals of Catalysis V	DLCC	316

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An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.

# 2018 TECHNICAL PROGRAM GRID

## 21 - Computational Molecular Science and Engineering Forum

Day	Time	Session #	Session Title	Property	Room
Sunday	8:00 AM	1	Workshop: Hands On With Molecular Simulation (Ticketed Event)	DLCC	334
Sunday	3:30 PM	13	Applications of Molecular Modeling to Study Interfacial Phenomena I	DLCC	308
Monday	8:00 AM	91	In Honor of Pablo Debenedetti I (Invited Talks)	DLCC	308
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	156	Industrial Applications of Computational Chemistry and Molecular Simulation	DLCC	308
Monday	12:30 PM	159	In Honor of Pablo Debenedetti II (Invited Talks)*	DLCC	307
Monday	12:30 PM	169	New Developments in Computational Catalysis I*	DLCC	402
Monday	3:30 PM	189	Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)	DLCC	Exhibit Hall B
Monday	3:30 PM	220	Faculty Candidates in CoMSEF	DLCC	308
Monday	3:30 PM	234	New Developments in Computational Catalysis II*	DLCC	402
Tuesday	8:00 AM	269	Computational Catalysis I: Fundamentals*	DLCC	402
Tuesday	8:00 AM	272	Data Mining and Machine Learning in Molecular Sciences I	DLCC	308
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	318	Applications of Molecular Modeling to Study Interfacial Phenomena II	DLCC	308
Tuesday	12:30 PM	327	Computational Catalysis II: Metal and Alloy Catalysis*	DLCC	402
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	389	Computational Catalysis III: Electrocatalysis*	DLCC	402
Tuesday	3:30 PM	403	Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)	DLCC	308
Tuesday	3:30 PM	429	Tools for Product Design*	DLCC	319
Wednesday	8:00 AM	448	Computational Catalysis IV: Biomass Chemistry and Chemicals Production*	DLCC	402
Wednesday	8:00 AM	449	Data-Driven Screening of Chemical and Materials Space*	DLCC	307
Wednesday	8:00 AM	476	Recent Advances in Molecular Simulation Methods I	DLCC	308
Wednesday	12:30 PM	504	Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, and Supported Catalysts*	DLCC	402
Wednesday	12:30 PM	532	Practical Applications of Computational Chemistry and Molecular Simulation	DLCC	308
Wednesday	3:30 PM	588	The Industrial Fluid Properties Simulation Challenge	DLCC	308
Thursday	8:00 AM	611	Data Mining and Machine Learning in Molecular Sciences II	DLCC	308
Thursday	12:30 PM	648	Atomistic and Molecular Modeling and Simulation of Polymers*	DLCC	330
Thursday	12:30 PM	659	Data Science in Catalysis I*	DLCC	402
Thursday	12:30 PM	671	Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction*	DLCC	307
Thursday	12:30 PM	683	Software Engineering in and for the Molecular Sciences	DLCC	308
Thursday	3:30 PM	699	Data Science in Catalysis II*	DLCC	402

\* This session is co-sponsored by one or more programming groups



# 2018 TECHNICAL PROGRAM GRID

## 21 - Computational Molecular Science and Engineering Forum

Day	Time	Session #	Session Title	Property	Room
Thursday	3:30 PM	710	Making Molecular Simulation a Mainstream Chemical Engineering Tool	DLCC	308
Friday	8:00 AM	739	Recent Advances in Molecular Simulation Methods II	DLCC	305
Friday	12:30 PM	750	Recent Advances in Force Fields*	DLCC	306

## 22 - Nanoscale Science and Engineering Forum

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	38	Nanofabrication and Nanoscale Processing I	DLCC	310
Monday	8:30 AM	110	Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks)	DLCC	310
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	167	Nanofabrication and Nanoscale Processing II	DLCC	310
Monday	3:30 PM	198	Poster Session: Nanoscale Science and Engineering	DLCC	Exhibit Hall B
Tuesday	8:00 AM	283	Environmental Applications of Nanotechnology and Nanomaterials*	DLCC	309
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	338	Environmental Implications of Nanomaterials: Biological Interactions*	DLCC	309
Tuesday	12:30 PM	340	Functional Nanoparticles*	DLCC	413
Tuesday	12:30 PM	363	Self and Directed Assembly at the Nanoscale I	DLCC	311
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	405	Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles*	DLCC	413
Tuesday	3:30 PM	416	Nanoparticles and Health*	DLCC	309
Tuesday	3:30 PM	420	Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)*	Westin	Pennsylvania East
Tuesday	3:30 PM	423	Self and Directed Assembly at the Nanoscale II	DLCC	311
Wednesday	12:30 PM	524	Nanoscale Phenomena in Macromolecular Systems*	DLCC	327
Wednesday	3:30 PM	573	Nanoscale Structure in Polymers*	DLCC	327
Thursday	8:00 AM	630	Novel Nanoparticles and Nanostructured Materials for Energy Applications*	DLCC	413

## 22A - Carbon Nanomaterials

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	135	Carbon Nanomaterials Graduate Student Award Session	DLCC	311
Tuesday	8:00 AM	286	Graphene and Carbon Nanotubes: Absorption, Separations, and Transport Processes	DLCC	310
Tuesday	12:30 PM	323	Carbon Nanofibers and Related Structures from Renewable and/or Cheap Feedstock and Their Applications	DLCC	310

\* This session is co-sponsored by one or more programming groups



Please refrain from photographing slides or taking video of sessions and presentations.

# 2018 TECHNICAL PROGRAM GRID

## 22A - Carbon Nanomaterials

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:30 AM	484	Area Plenary: Carbon Nanomaterials (Invited Talks)	DLCC	310
Wednesday	12:30 PM	515	Graphene 2-D Materials: Synthesis, Functions and Applications I	DLCC	310
Wednesday	3:30 PM	566	Graphene 2-D Materials: Synthesis, Functions and Applications II	DLCC	310
Thursday	12:30 PM	666	Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion I	DLCC	310
Thursday	3:30 PM	706	Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion II	DLCC	310

## 22B - Bionanotechnology

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	39	Nanostructured Biomimetic and Biohybrid Materials and Devices	DLCC	311
Monday	8:00 AM	66	Biotechnology & Materials U.G. Research Session (Invited Talks)*	DLCC	302
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research*	Westin	Pennsylvania East
Tuesday	8:00 AM	261	Area Plenary: Bionanotechnology (Invited Talks)	DLCC	311
Tuesday	12:30 PM	319	Biocolloids, Biomolecules, and Nanomaterials of Medical Relevance *	Westin	Pennsylvania East
Tuesday	12:30 PM	338	Environmental Implications of Nanomaterials: Biological Interactions*	DLCC	309
Tuesday	12:30 PM	353	Nucleic Acid Materials and Delivery*	DLCC	328
Tuesday	3:30 PM	387	Bionanotechnology Graduate Student Award Session	DLCC	310
Tuesday	3:30 PM	420	Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)*	Westin	Pennsylvania East
Wednesday	12:30 PM	496	Biomaterial Scaffolds for Tissue Engineering I: Musculoskeletal Applications*	DLCC	328
Wednesday	12:30 PM	498	Bionanotechnology for Gene and Drug Delivery I	DLCC	309
Wednesday	12:30 PM	525	Nanotechnology for Biotechnology and Pharmaceuticals I	DLCC	311
Wednesday	3:30 PM	554	Biomaterial Scaffolds for Tissue Engineering II: Bioactive and Drug-Eluting Materials*	DLCC	328
Wednesday	3:30 PM	555	Bionanotechnology for Gene and Drug Delivery II	DLCC	309
Wednesday	3:30 PM	575	Nanotechnology for Biotechnology and Pharmaceuticals II	DLCC	311
Thursday	8:00 AM	636	Self-Assembled Biomaterials	DLCC	311
Thursday	12:30 PM	676	Nanobiotechnology for Sensors and Imaging I	DLCC	311
Thursday	3:30 PM	712	Nanobiotechnology for Sensors and Imaging II	DLCC	311

## 23 - Sustainable Engineering Forum

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	16	Biobased Intermediates and Biomaterials*	DLCC	335
Sunday	3:30 PM	30	Fundamentals of Food, Energy, and Water Systems*	DLCC	320
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317
Monday	8:00 AM	86	Fundamentals of Environmental Kinetics and Reaction Engineering*	DLCC	320

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## 23 - Sustainable Engineering Forum

Day	Time	Session #	Session Title	Property	Room
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	151	FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)*	DLCC	317
Monday	12:30 PM	174	Solar Energy for Power Generation and Chemical Processing I*	DLCC	324
Monday	3:30 PM	243	Solar Energy for Power Generation and Chemical Processing II*	DLCC	324
Monday	3:30 PM	246	World Cafe: Food-Energy-Water Nexus (Invited Talks and Panel Discussion)*	DLCC	317
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	322	Breakthroughs in C1 to Chemicals and Processing Engineering*	DLCC	318
Tuesday	12:30 PM	365	Sustainable and Green Product Design*	DLCC	319
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	408	Integrated Process Engineering and Economic Analysis*	DLCC	318
Wednesday	8:00 AM	445	Catalysis for C1 Chemistry I: Methanol Formation and Upgrading*	DLCC	403
Wednesday	8:00 AM	458	Forum Plenary: Sustainable Engineering Forum (Invited Talks)	DLCC	315
Wednesday	12:30 PM	500	Catalysis for C1 Chemistry II: Methane Reforming and Oxidation*	DLCC	403
Thursday	8:00 AM	605	Catalysis for C1 Chemistry III: Methane and CO <sub>2</sub> *	DLCC	403
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols*	DLCC	405
Thursday	2:30 PM	761	Workshop on Identifying the Gaps and Opportunities in Graduate Education to Improve Sustainability of the US Chemical Industries	DLCC	318
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin*	DLCC	405
Thursday	3:30 PM	705	Fundamentals of Sustainability Science and Engineering*	DLCC	319
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry*	DLCC	315
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks*	DLCC	315

## 23A - General

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	23	Chemical Engineers for a World of Good: Bringing Hard and Soft Engineering Skills and Sustainability to Undergraduates	DLCC	315
Monday	8:00 AM	62	Big Data and Sustainability	DLCC	315
Monday	8:00 AM	100	Process Research for Improved Throughput & Efficiency, and Reduced Cost & Environmental Impact*	DLCC	335
Monday	3:30 PM	223	Green Chemistry and Engineering	DLCC	309
Monday	3:30 PM	232	Nanomaterial Applications for Human Health and the Environment	DLCC	310
Tuesday	8:00 AM	303	Sustainable Management and Uses of Post-Consumer Materials and Waste	DLCC	315
Tuesday	12:30 PM	366	The Food-Energy-Water Nexus	DLCC	315

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# 2018 TECHNICAL PROGRAM GRID

## 23A - General

Day	Time	Session #	Session Title	Property	Room
Tuesday	3:30 PM	401	Emerging Trends in Life Cycle Analysis	DLCC	315
Wednesday	8:00 AM	440	Advances in Industrial Modeling & Optimization: Methodologies, Tools and Applications*	DLCC	335
Wednesday	12:30 PM	536	Safety and Sustainability Best Practices	DLCC	315
Wednesday	3:30 PM	548	Poster Session: Sustainability and Sustainable Biorefineries	DLCC	Exhibit Hall B
Thursday	12:30 PM	682	Process Design: Innovation for Sustainability	DLCC	316

## 23B - Sustainable Biorefineries

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	16	Biobased Intermediates and Biomaterials*	DLCC	335
Sunday	3:30 PM	27	Feedstock Logistics for Biorefineries	DLCC	316
Sunday	3:30 PM	48	Reactor Engineering for Biomass Feedstocks	DLCC	317
Monday	8:00 AM	92	Integrating Municipal and Industrial Waste into Biorefineries	DLCC	316
Monday	12:30 PM	125	Advances in Algal Biorefineries I	DLCC	315
Monday	12:30 PM	132	Area Plenary: Sustainable Biorefineries (Invited Talks)	DLCC	316
Monday	3:30 PM	204	Advances in Algal Biorefineries II	DLCC	315
Monday	3:30 PM	210	Chemical and Catalytic Conversions and Processes for Renewable Feedstocks	DLCC	316
Tuesday	8:00 AM	254	Advances in Enzymatic Catalysis I*	DLCC	405
Tuesday	8:00 AM	263	Biofuels Production: Design, Simulation, and Economic Analysis	DLCC	316
Tuesday	12:30 PM	316	Advances in Enzymatic Catalysis II*	DLCC	405
Tuesday	12:30 PM	346	Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals	DLCC	316
Tuesday	3:30 PM	395	Developments in Biorefineries	DLCC	316
Tuesday	3:30 PM	424	Separation Processes in Biorefineries*	DLCC	324
Wednesday	8:00 AM	482	USA-China Progress in Biomass Conversion Technologies I*	DLCC	325
Wednesday	12:30 PM	495	Biomass Thermal Deconstruction via Fast Pyrolysis Biorefineries	DLCC	316
Wednesday	12:30 PM	540	USA-China Progress in Biomass Conversion Technology II*	DLCC	325
Wednesday	3:30 PM	591	USA-China Progress in Biomass Conversion Technology III*	DLCC	325
Thursday	8:00 AM	602	Biological Conversions and Processes for Renewable Feedstocks	DLCC	316
Thursday	8:00 AM	635	Recalcitrance of Woody Biomass*	DLCC	324
Thursday	8:00 AM	640	Thermochemical Conversion of Biomass*	DLCC	325
Thursday	12:30 PM	649	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries I*	DLCC	325
Thursday	12:30 PM	651	Biomass Characterization, Pretreatment, and Fractionation I*	DLCC	324
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols*	DLCC	405
Thursday	3:30 PM	690	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries II*	DLCC	325
Thursday	3:30 PM	691	Biomass Characterization, Pretreatment, and Fractionation II*	DLCC	324

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# 2018 TECHNICAL PROGRAM GRID

## 23B - Sustainable Biorefineries

Day	Time	Session #	Session Title	Property	Room
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin*	DLCC	405
Thursday	3:30 PM	726	Value-Added Co-Products from Biorefineries	DLCC	316
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry*	DLCC	315
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks*	DLCC	315

## 23C - Sustainable Energy

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	79	Electrocatalysis and Photoelectrocatalysis I: Fundamentals of CO <sub>2</sub> Reduction *	DLCC	401
Monday	12:30 PM	145	Electrocatalysis and Photoelectrocatalysis II: Reactors and Processes for CO <sub>2</sub> Reduction*	DLCC	401
Monday	12:30 PM	146	Energy & the Environment U.G. Research Session (Invited Talks)*	DLCC	302
Monday	3:30 PM	217	Electrocatalysis and Photoelectrocatalysis III: Hydrogen Evolution Reaction*	DLCC	401
Tuesday	8:00 AM	304	The Energy-Water Nexus	DLCC	317
Tuesday	12:30 PM	331	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I	DLCC	317
Tuesday	3:30 PM	394	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II	DLCC	317
Thursday	8:00 AM	613	Distributed Chemical and Energy Processes for Sustainability	DLCC	317
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols*	DLCC	405
Thursday	12:30 PM	661	Energy Sustainability: Challenges and Solutions	DLCC	317
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin*	DLCC	405
Thursday	3:30 PM	724	Sustainable Energy: Generation and Storage	DLCC	317
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry*	DLCC	315
Friday	8:00 AM	733	Modeling and Computation in Energy and Environment*	DLCC	310
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks*	DLCC	315

\* This session is co-sponsored by one or more programming groups

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# 2018 TECHNICAL PROGRAM GRID

## 24 - Chemical Engineering & the Law Forum

Day	Time	Session #	Session Title	Property	Room
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	161	Intellectual Property for Practicing Engineers: Patents and Trade Secrets	DLCC	320
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303

## 25 - Upstream Engineering and Flow Assurance Forum

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	85	Fundamentals and Applications of Flow Assurance	DLCC	305
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	152	Flow Assurance and Asset Integrity	DLCC	305
Monday	3:30 PM	201	Poster Session: Upstream Engineering and Flow Assurance	DLCC	Exhibit Hall B
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Friday	12:30 PM	746	Gas Hydrates Science and Engineering*	DLCC	307

## 26 - Pharmaceutical Discovery, Development and Manufacturing Forum

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	15	Automation and High-Throughput Technologies for Pharmaceutical Discovery and Development	Westin	Fayette
Sunday	3:30 PM	31	Green Chemical Reaction Engineering for Sustainability*	DLCC	401
Sunday	3:30 PM	34	Innovations in Pharmaceutical Discovery, Development, and Manufacturing	Westin	Washington
Monday	8:00 AM	56	3D Printing II*	DLCC	333
Monday	8:00 AM	81	Forum Plenary: Pharmaceutical Discovery, Development, and Manufacturing Forum (Invited Talks)	Westin	Allegheny Grand Ballroom II
Monday	8:00 AM	102	Reaction Engineering in Pharmaceuticals and Fine Chemicals*	DLCC	404
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	123	3D Printing Keynote (Invited Talks)*	DLCC	333
Monday	12:30 PM	139	Computational Solid State Pharmaceutics	Westin	Washington
Monday	12:30 PM	141	Data Analytics in Operational Support	Westin	Fayette
Monday	12:30 PM	160	In Honor of the 2017 Wilhelm Award Winner I (Invited Talks)*	DLCC	406
Monday	12:30 PM	171	Pharmaceutical Process Development and Pilot Plants*	DLCC	336
Monday	12:30 PM	314	Advancements in Materials Science for Powder Handling in Pharmaceutical Process Development	Westin	Cambria

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# 2018 TECHNICAL PROGRAM GRID

## 26 - Pharmaceutical Discovery, Development and Manufacturing Forum

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	200	Poster Session: Pharmaceutical	DLCC	Exhibit Hall B
Monday	6:30 PM	250	Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony	Westin	Allegheny Grand Ballroom II
Tuesday	8:00 AM	252	Advancements in Polymers and Amorphous Solids for Pharmaceutical Process Development	Westin	Fayette
Tuesday	8:00 AM	254	Advances in Enzymatic Catalysis I*	DLCC	405
Tuesday	8:00 AM	264	Biomaterials for Drug Delivery*	DLCC	328
Tuesday	8:00 AM	270	Continuous Crystallization Processes*	DLCC	302
Tuesday	8:00 AM	281	Emerging Technologies in Pharmaceutical Research and Manufacturing	Westin	Washington
Tuesday	8:00 AM	289	In Honor of Professor D. Ramkrishna's Contributions to Biopharmaceutical Industry (Invited Talks)	Westin	Somerset
Tuesday	8:00 AM	299	Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries*	DLCC	404
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	140	Data Analytics for Process Prediction	Westin	Fayette
Tuesday	12:30 PM	316	Advances in Enzymatic Catalysis II*	DLCC	405
Tuesday	12:30 PM	328	Continuous Processing Technologies Applied in Drug Substance Manufacturing I	Westin	Somerset
Tuesday	12:30 PM	330	Crystallization of Pharmaceutical and Biological Molecules*	DLCC	302
Tuesday	12:30 PM	336	Enabling and Advanced Formulations in Drug Product Processing I: Focus on Dissolution	Westin	Washington
Tuesday	3:30 PM	381	Advancements in Particle Engineering for Crystallization in Pharmaceutical Process Development	Westin	Fayette
Tuesday	3:30 PM	384	AIChE's 110 Year Celebration (Invited Talks)*	DLCC	303
Tuesday	3:30 PM	391	Continuous Processing Technologies Applied in Drug Substance Manufacturing II	Westin	Somerset
Tuesday	3:30 PM	398	Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)*	Westin	Allegheny Grand Ballroom II
Tuesday	3:30 PM	402	Enabling and Advanced Formulations in Drug Product Processing II: Focus on Stability	Westin	Washington
Wednesday	8:00 AM	466	Mixing Scale-up/Scale-down Issues in Pharmaceutical and Biopharmaceuticals Processes*	DLCC	334
Wednesday	8:00 AM	468	Modeling and Control of Crystallization*	DLCC	302
Wednesday	8:00 AM	470	Multivariate Experimentation and Modeling for Pharmaceutical Products and Processes	Westin	Fayette

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# 2018 TECHNICAL PROGRAM GRID

## 26 - Pharmaceutical Discovery, Development and Manufacturing Forum

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	470	Multivariate Experimentation and Modeling for Pharmaceutical Products and Processes	Westin	Fayette
Wednesday	8:00 AM	473	Panel: Pharmaceutical Engineering Challenges As Approached By Chemical Engineers Outside of Pharma (Invited Talks)	Westin	Somerset
Wednesday	12:30 PM	505	Continuous Processing Technologies Applied in Drug Product Development I	Westin	Washington
Wednesday	12:30 PM	507	Developing Process Control Strategies for Drug Product Manufacture	Westin	Fayette
Wednesday	3:30 PM	557	Continuous Processing Technologies Applied in Drug Product Development II	Westin	Washington
Wednesday	3:30 PM	558	Developing Process Control Strategies for Drug Substance Manufacture	Westin	Fayette
Thursday	8:00 AM	621	Innovations in Process Analytical Technology (PAT) and In Situ Analysis	Westin	Somerset
Thursday	8:00 AM	626	Mechanistic Models for Integrated Pharmaceutical Product and Process Design	Westin	Fayette
Thursday	12:30 PM	645	Application of Process Modelling to Pharmaceutical Process Design and Scale-up	Westin	Fayette
Thursday	12:30 PM	667	Innovative Technologies to Accelerate and Enhance Drug Discovery, Development, and Manufacturing	Westin	Somerset
Thursday	12:30 PM	678	Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications I*	DLCC	413
Thursday	12:30 PM	684	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond I*	DLCC	302
Thursday	3:30 PM	697	Control Strategy Development for Continuous Drug Substance and Drug Product Manufacture	Westin	Somerset
Thursday	3:30 PM	714	Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications II*	DLCC	413
Thursday	3:30 PM	719	Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals	Westin	Fayette
Thursday	3:30 PM	723	Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond II*	DLCC	302
Friday	8:00 AM	737	Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions*	DLCC	302

## POSTERSESSIONS - Poster Sessions

Day	Time	Session #	Session Title	Property	Room
Sunday	1:00 PM	6	Meet the Faculty Candidate Poster Session*	DLCC	Exhibit Hall B
Monday	3:30 PM	182	Interactive Session: Applied Mathematics and Numerical Analysis*	DLCC	Exhibit Hall B
Monday	3:30 PM	183	Interactive Session: Data and Information Systems*	DLCC	Exhibit Hall B
Monday	3:30 PM	184	Interactive Session: Systems and Process Control*	DLCC	Exhibit Hall B
Monday	3:30 PM	185	Interactive Session: Systems and Process Design*	DLCC	Exhibit Hall B
Monday	3:30 PM	186	Interactive Session: Systems and Process Operations*	DLCC	Exhibit Hall B
Monday	3:30 PM	187	Poster Session: Advances in Fossil Energy R&D*	DLCC	Exhibit Hall B

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# 2018 TECHNICAL PROGRAM GRID

## Poster Sessions

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	188	Poster Session: Bioengineering*	DLCC	Exhibit Hall B
Monday	3:30 PM	189	Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)*	DLCC	Exhibit Hall B
Monday	3:30 PM	190	Poster Session: Engineering Fundamentals in Life Science *	DLCC	Exhibit Hall B
Monday	3:30 PM	192	Poster Session: Interfacial Phenomena (Area 1C)*	DLCC	Exhibit Hall B
Monday	3:30 PM	193	Poster Session: Materials Engineering & Sciences (08A - Polymers)*	DLCC	Exhibit Hall B
Monday	3:30 PM	194	Poster Session: Materials Engineering & Sciences (08B - Biomaterials)*	DLCC	Exhibit Hall B
Monday	3:30 PM	195	Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)*	DLCC	Exhibit Hall B
Monday	3:30 PM	196	Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)*	DLCC	Exhibit Hall B
Monday	3:30 PM	197	Poster Session: Materials Engineering & Sciences (08F - Composite Materials)*	DLCC	Exhibit Hall B
Monday	3:30 PM	198	Poster Session: Nanoscale Science and Engineering*	DLCC	Exhibit Hall B
Monday	3:30 PM	199	Poster Session: Novel Products from Forest and Plant Biomass*	DLCC	Exhibit Hall B
Monday	3:30 PM	200	Poster Session: Pharmaceutical*	DLCC	Exhibit Hall B
Monday	3:30 PM	201	Poster Session: Upstream Engineering and Flow Assurance*	DLCC	Exhibit Hall B
Monday	3:30 PM	237	Poster Session: Fluid Mechanics*	Omni	Frick
Tuesday	3:30 PM	372	Poster Session: Chemical Engineering Education*	DLCC	Exhibit Hall B
Tuesday	3:30 PM	373	Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange*	DLCC	Exhibit Hall B
Tuesday	3:30 PM	374	Poster Session: General Topics on Separations *	DLCC	Exhibit Hall B
Tuesday	3:30 PM	375	Poster Session: Particle Technology Forum*	DLCC	Exhibit Hall B
Tuesday	3:30 PM	376	Poster Session: Separations Division*	DLCC	Exhibit Hall B
Tuesday	3:30 PM	377	Poster Session: Thermodynamics and Transport Properties (Area 1A)*	DLCC	Exhibit Hall B
Tuesday	3:30 PM	378	Poster Session: Transport and Energy Processes*	DLCC	Exhibit Hall B
Wednesday	3:30 PM	544	Poster Session: Catalysis and Reaction Engineering (CRE) Division*	DLCC	Exhibit Hall B
Wednesday	3:30 PM	545	Poster Session: Environmental Division*	DLCC	Exhibit Hall B
Wednesday	3:30 PM	546	Poster Session: Fuels and Petrochemicals Division*	DLCC	Exhibit Hall B
Wednesday	3:30 PM	547	Poster Session: Process Development*	DLCC	Exhibit Hall B
Wednesday	3:30 PM	548	Poster Session: Sustainability and Sustainable Biorefineries*	DLCC	Exhibit Hall B
Wednesday	5:30 PM	593	Poster Session: NH3 Energy+ Technologies*	DLCC	318

## T1 - Meet the Faculty Candidate Poster Session – Sponsored by the Education Division

Day	Time	Session #	Session Title	Property	Room
Sunday	10:00 AM	4	Workshop: Career Planning for Prospective Faculty*	DLCC	408
Sunday	1:00 PM	6	Meet the Faculty Candidate Poster Session	DLCC	Exhibit Hall B
Sunday	3:30 PM	55	Workshop: Effective Teaching for New or Prospective Faculty*	DLCC	411

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# 2018 TECHNICAL PROGRAM GRID

## T1 - Meet the Faculty Candidate Poster Session – Sponsored by the Education Division

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	65	Biomaterials and Life Science Engineering: Faculty Candidates*	DLCC	328
Monday	3:30 PM	220	Faculty Candidates in CoMSEF*	DLCC	308
Tuesday	12:30 PM	335	Electrochemical Fundamentals: Faculty Candidate Session*	DLCC	306

## T4A - Biorefinery Technologies for Forest Based Lignocellulosic Biomass

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	27	Feedstock Logistics for Biorefineries*	DLCC	316
Sunday	3:30 PM	48	Reactor Engineering for Biomass Feedstocks*	DLCC	317
Monday	8:00 AM	63	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion*	Westin	Westmoreland West-Central
Monday	8:00 AM	92	Integrating Municipal and Industrial Waste into Biorefineries*	DLCC	316
Monday	12:30 PM	125	Advances in Algal Biorefineries I*	DLCC	315
Monday	12:30 PM	132	Area Plenary: Sustainable Biorefineries (Invited Talks)*	DLCC	316
Monday	12:30 PM	144	Efficient Processing of Lignin to Bioproducts and Biofuels I*	DLCC	318
Monday	3:30 PM	204	Advances in Algal Biorefineries II*	DLCC	315
Monday	3:30 PM	210	Chemical and Catalytic Conversions and Processes for Renewable Feedstocks*	DLCC	316
Monday	3:30 PM	216	Efficient Processing of Lignin to Bioproducts and Biofuels II*	DLCC	318
Tuesday	8:00 AM	263	Biofuels Production: Design, Simulation, and Economic Analysis*	DLCC	316
Tuesday	12:30 PM	346	Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals*	DLCC	316
Tuesday	3:30 PM	395	Developments in Biorefineries*	DLCC	316
Tuesday	3:30 PM	424	Separation Processes in Biorefineries	DLCC	324
Wednesday	8:00 AM	458	Forum Plenary: Sustainable Engineering Forum (Invited Talks)*	DLCC	315
Wednesday	8:00 AM	475	Reaction Engineering for Biomass Conversion I*	DLCC	401
Wednesday	8:00 AM	482	USA-China Progress in Biomass Conversion Technologies I	DLCC	325
Wednesday	12:30 PM	495	Biomass Thermal Deconstruction via Fast Pyrolysis Biorefineries*	DLCC	316
Wednesday	12:30 PM	535	Reaction Engineering for Biomass Conversion II*	DLCC	401
Wednesday	12:30 PM	540	USA-China Progress in Biomass Conversion Technology II	DLCC	325
Wednesday	3:30 PM	548	Poster Session: Sustainability and Sustainable Biorefineries*	DLCC	Exhibit Hall B
Wednesday	3:30 PM	591	USA-China Progress in Biomass Conversion Technology III	DLCC	325
Thursday	8:00 AM	602	Biological Conversions and Processes for Renewable Feedstocks*	DLCC	316
Thursday	8:00 AM	635	Recalcitrance of Woody Biomass	DLCC	324
Thursday	8:00 AM	640	Thermochemical Conversion of Biomass	DLCC	325
Thursday	12:30 PM	649	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries I	DLCC	325
Thursday	12:30 PM	651	Biomass Characterization, Pretreatment, and Fractionation I	DLCC	324

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# 2018 TECHNICAL PROGRAM GRID

## T4A - Biorefinery Technologies for Forest Based Lignocellulosic Biomass

Day	Time	Session #	Session Title	Property	Room
Thursday	12:30 PM	649	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries I	DLCC	325
Thursday	12:30 PM	651	Biomass Characterization, Pretreatment, and Fractionation I	DLCC	324
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols*	DLCC	405
Thursday	3:30 PM	690	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries II	DLCC	325
Thursday	3:30 PM	691	Biomass Characterization, Pretreatment, and Fractionation II	DLCC	324
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin*	DLCC	405
Thursday	3:30 PM	726	Value-Added Co-Products from Biorefineries*	DLCC	316
Friday	8:00 AM	729	Bio-Based Polymers*	DLCC	319
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry*	DLCC	315
Friday	8:00 AM	738	Pyrolysis of Biomass*	DLCC	317
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks*	DLCC	315

## T4B - Solar Energy for Power Generation and Chemical Processing

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	79	Electrocatalysis and Photoelectrocatalysis I: Fundamentals of CO <sub>2</sub> Reduction *	DLCC	401
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	145	Electrocatalysis and Photoelectrocatalysis II: Reactors and Processes for CO <sub>2</sub> Reduction*	DLCC	401
Monday	12:30 PM	174	Solar Energy for Power Generation and Chemical Processing I	DLCC	324
Monday	3:30 PM	217	Electrocatalysis and Photoelectrocatalysis III: Hydrogen Evolution Reaction*	DLCC	401
Monday	3:30 PM	243	Solar Energy for Power Generation and Chemical Processing II	DLCC	324
Tuesday	8:00 AM	280	Electrocatalysis and Photoelectrocatalysis IV: Advances in Fuel Cell Catalysts*	DLCC	401
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	334	Electrocatalysis and Photoelectrocatalysis V: Oxygen Evolution Reaction*	DLCC	401
Tuesday	3:30 PM	399	Electrocatalysis and Photoelectrocatalysis VI: Biomass Processing and Ammonia Synthesis*	DLCC	401
Tuesday	3:30 PM	408	Integrated Process Engineering and Economic Analysis*	DLCC	318
Tuesday	3:30 PM	418	Nuclear Applications of Electrochemical Engineering*	DLCC	326
Thursday	3:30 PM	724	Sustainable Energy: Generation and Storage *	DLCC	317
Friday	8:00 AM	734	Modeling, Control, and Optimization of Energy Systems *	DLCC	309

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## T4C - Hydrogen Production and Storage

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	25	Electrochemical Storage Materials and Devices*	DLCC	330
Tuesday	8:00 AM	259	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas*	DLCC	324
Wednesday	8:00 AM	453	Electrochemical Reactors, Fuel Cells, and Electrolyzers I*	DLCC	323
Wednesday	12:30 PM	490	Advanced Fuel Cell, Hydrogen Generation & Storage Technologies*	DLCC	324
Wednesday	12:30 PM	511	Electrochemical Reactors, Fuel Cells, and Electrolyzers II*	DLCC	323
Wednesday	12:30 PM	514	Fuel Processing for Hydrogen Production*	DLCC	321
Wednesday	3:30 PM	562	Electronic and Photonic Materials Devices and Theory*	DLCC	330
Thursday	12:30 PM	680	Polymers for Energy Storage and Conversion*	DLCC	327

## T4E - Alternative Energy & Enabling Technologies

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	48	Reactor Engineering for Biomass Feedstocks*	DLCC	317
Monday	8:00 AM	63	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion*	Westin	Westmoreland West-Central
Monday	3:30 PM	206	Alternative Fuels*	DLCC	405
Tuesday	8:00 AM	259	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas*	DLCC	324
Wednesday	8:00 AM	453	Electrochemical Reactors, Fuel Cells, and Electrolyzers I*	DLCC	323
Wednesday	8:00 AM	482	USA-China Progress in Biomass Conversion Technologies I*	DLCC	325
Wednesday	12:30 PM	511	Electrochemical Reactors, Fuel Cells, and Electrolyzers II*	DLCC	323
Wednesday	3:30 PM	574	Nanostructured Thin Films*	DLCC	329
Thursday	8:00 AM	599	Alternative Fuels and Enabling Technologies I*	DLCC	323
Thursday	8:00 AM	640	Thermochemical Conversion of Biomass*	DLCC	325
Thursday	12:30 PM	680	Polymers for Energy Storage and Conversion*	DLCC	327
Thursday	3:30 PM	724	Sustainable Energy: Generation and Storage *	DLCC	317

## T4F - BioFuels

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	63	Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion*	Westin	Westmoreland West-Central
Monday	12:30 PM	142	Developments in Petroleum and Biofuels Refining Technologies *	DLCC	323
Tuesday	8:00 AM	259	Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas*	DLCC	324
Wednesday	8:00 AM	453	Electrochemical Reactors, Fuel Cells, and Electrolyzers I*	DLCC	323
Wednesday	8:00 AM	482	USA-China Progress in Biomass Conversion Technologies I*	DLCC	325
Wednesday	12:30 PM	511	Electrochemical Reactors, Fuel Cells, and Electrolyzers II*	DLCC	323
Wednesday	12:30 PM	525	Nanotechnology for Biotechnology and Pharmaceuticals I*	DLCC	311

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# 2018 TECHNICAL PROGRAM GRID

T4F - BioFuels					
Day	Time	Session #	Session Title	Property	Room
Wednesday	12:30 PM	540	USA-China Progress in Biomass Conversion Technology II*	DLCC	325
Wednesday	3:30 PM	591	USA-China Progress in Biomass Conversion Technology III*	DLCC	325
Thursday	8:00 AM	640	Thermochemical Conversion of Biomass*	DLCC	325
Thursday	12:30 PM	649	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries I*	DLCC	325
Thursday	12:30 PM	651	Biomass Characterization, Pretreatment, and Fractionation I*	DLCC	324
Thursday	3:30 PM	690	Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries II*	DLCC	325

T4G - Fossil Fuels & CCS					
Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	11	Advanced Materials for Carbon Dioxide Capture for Power Generation *	DLCC	321
Sunday	3:30 PM	46	Reaction Engineering for Combustion and Pyrolysis*	DLCC	402
Monday	8:00 AM	73	Combustion Kinetics and Emissions*	DLCC	402
Monday	12:30 PM	147	Engineering Geologic Carbon Dioxide Storage Systems*	DLCC	321
Monday	3:30 PM	235	Novel Approaches to CO <sub>2</sub> Utilization*	DLCC	321
Tuesday	8:00 AM	274	Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems*	DLCC	321
Tuesday	12:30 PM	329	CO <sub>2</sub> Capture, Utilization, and Disposal: Key to Clean Energy Production*	DLCC	324
Tuesday	12:30 PM	370	Value-Added Chemicals from Natural Gas*	DLCC	321
Wednesday	8:00 AM	445	Catalysis for C1 Chemistry I: Methanol Formation and Upgrading*	DLCC	403
Wednesday	12:30 PM	506	CO <sub>2</sub> Capture By Adsorption*	DLCC	334
Thursday	8:00 AM	633	Rare Earth Elements: Extraction, Separation, Characterization, Economics, Criticality, and Kinetics*	DLCC	321
Thursday	12:30 PM	677	New Technologies to Enhance the Production of Unconventional Oil and Natural Gas: Experimentation*	DLCC	321

T4H - International Congress on Energy (ICE) 2018					
Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	11	Advanced Materials for Carbon Dioxide Capture for Power Generation *	DLCC	321
Sunday	4:15 PM	22	Chemical Engineering in Sustainability (YCOSST) and Policy (WISE) Award Recipient Talks (Invited Talks)*	DLCC	307
Tuesday	3:30 PM	430	Topical Plenary: Advances in Fossil Energy R&D (Invited Talks)*	DLCC	321

T5 - Nanomaterials for Applications in Energy and Biology					
Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	29	Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic and Photoelectrochemical Reactions	DLCC	412
Monday	8:00 AM	96	Nanomaterials for Biological Application I	DLCC	412

\* This session is co-sponsored by one or more programming groups

# 2018 TECHNICAL PROGRAM GRID

## T5 - Nanomaterials for Applications in Energy and Biology

Day	Time	Session #	Session Title	Property	Room
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	168	Nanomaterials for Biological Application II	DLCC	412
Monday	3:30 PM	233	Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon	DLCC	412
Tuesday	8:00 AM	283	Environmental Applications of Nanotechnology and Nanomaterials*	DLCC	309
Tuesday	8:00 AM	294	Nanomaterials for Energy Storage I	DLCC	412
Tuesday	8:00 AM	296	Novel Nanostructured Catalytic Materials I*	DLCC	403
Tuesday	12:30 PM	338	Environmental Implications of Nanomaterials: Biological Interactions*	DLCC	309
Tuesday	12:30 PM	352	Novel Nanostructured Catalytic Materials II*	DLCC	403
Tuesday	3:30 PM	415	Nanomaterials for Energy Storage II	DLCC	412
Wednesday	8:00 AM	471	Nanomaterials for Hydrogen Production and Fuel Cells I	DLCC	412
Wednesday	12:30 PM	523	Nanomaterials for Hydrogen Production and Fuel Cells II	DLCC	412
Thursday	8:00 AM	637	Semiconducting Quantum Dots and Nanocrystals*	DLCC	330

## T6A - Next-Gen Manufacturing

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I*	DLCC	333
Monday	8:00 AM	56	3D Printing II*	DLCC	333
Monday	8:00 AM	64	Biomaterials*	DLCC	311
Monday	3:30 PM	218	Emerging Trends in Smart Manufacturing (sponsored by CESMII)	DLCC	408
Tuesday	8:00 AM	287	Industrial Internet of Things (IIoT) Applications and Industry 4.0 Forum	DLCC	333
Tuesday	12:30 PM	356	Polymers in Additive Manufacturing*	DLCC	333
Tuesday	3:30 PM	392	Cybersecurity	DLCC	333
Wednesday	8:00 AM	464	Membrane Reactors*	DLCC	304
Wednesday	11:15 AM	487	John M. Prausnitz AIChE Institute Lecture*	DLCC	Spirit of Pittsburgh A
Thursday	8:00 AM	613	Distributed Chemical and Energy Processes for Sustainability*	DLCC	317
Thursday	8:00 AM	629	Modeling, Control, and Optimization of Manufacturing Systems*	DLCC	408
Thursday	3:30 PM	692	Bioprinting of Scaffolds, Tissues, and Organs*	DLCC	328

## T6B - Process Intensification & Modular Chemical Processing

Day	Time	Session #	Session Title	Property	Room
Monday	3:30 PM	236	PI Topical Conference Plenary: A Look Inside the RAPID Manufacturing Institute, Co-Hosted by RAPID and F&PD	DLCC	335
Monday	5:50 PM	756	RAPID Manufacturing Institute Open House	DLCC	335
Tuesday	8:00 AM	258	Advances in Process Intensification*	DLCC	335
Tuesday	12:30 PM	360	Process Intensification By Enhanced Heat and Mass Transfer*	DLCC	335

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Baltimore, MD  
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# 2018 TECHNICAL PROGRAM GRID

## T6B - Process Intensification & Modular Chemical Processing

Day	Time	Session #	Session Title	Property	Room
Tuesday	3:30 PM	422	Process Intensification By Process Integration*	DLCC	335
Wednesday	8:00 AM	464	Membrane Reactors*	DLCC	304
Wednesday	11:15 AM	487	John M. Prausnitz AIChE Institute Lecture*	DLCC	Spirit of Pittsburgh A
Wednesday	12:30 PM	533	Process Intensification through the Application of Microreactors, Multiphase Reactors, and Membrane Reactors*	DLCC	335
Wednesday	3:30 PM	583	Process Intensification through Process Systems Engineering*	DLCC	409

## T6C - 3D Printing

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	9	3D Printing I	DLCC	333
Monday	8:00 AM	56	3D Printing II	DLCC	333
Monday	12:30 PM	123	3D Printing Keynote (Invited Talks)	DLCC	333
Monday	3:30 PM	202	3D Printing of Composites	DLCC	333
Tuesday	11:15 AM	312	Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture*	DLCC	Spirit of Pittsburgh A
Tuesday	12:30 PM	356	Polymers in Additive Manufacturing	DLCC	333
Wednesday	8:00 AM	435	Additive Manufacturing of Energetics*	DLCC	413
Thursday	3:30 PM	692	Bioprinting of Scaffolds, Tissues, and Organs*	DLCC	328

## T7 - The Food-Energy-Water Nexus

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	30	Fundamentals of Food, Energy, and Water Systems*	DLCC	320
Sunday	4:15 PM	22	Chemical Engineering in Sustainability (YCOST) and Policy (WISE) Award Recipient Talks (Invited Talks)*	DLCC	307
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)	DLCC	317
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	151	FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)	DLCC	317
Monday	3:30 PM	246	World Cafe: Food-Energy-Water Nexus (Invited Talks and Panel Discussion)	DLCC	317
Tuesday	8:00 AM	304	The Energy-Water Nexus*	DLCC	317
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	366	The Food-Energy-Water Nexus*	DLCC	315

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# 2018 TECHNICAL PROGRAM GRID

## T8 - Microbes at Biomedical Interfaces

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	107	Topical Plenary: Microbial Interaction with Biointerfaces (Invited Talks)	Westin	Pennsylvania East
Monday	10:00 AM	111	Microbes at Biomedical Interfaces Undergraduate Poster Competition*	DLCC	Exhibit Hall B
Monday	12:30 PM	154	Functional Interfaces to Control Pathogenic or Beneficial Microbes	Westin	Pennsylvania East
Monday	3:30 PM	222	Graduate Student Competition in Microbiointerface Research	Westin	Pennsylvania East
Tuesday	8:00 AM	279	Electroactive Biomaterials to Sense and Control Microbial Infections	Westin	Pennsylvania East
Tuesday	12:30 PM	319	Biocolloids, Biomolecules, and Nanomaterials of Medical Relevance	Westin	Pennsylvania East
Tuesday	3:30 PM	420	Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)	Westin	Pennsylvania East

## T9 - Sensors

Day	Time	Session #	Session Title	Property	Room
Monday	12:30 PM	134	Biosensors, Bidiagnosis and Bioprocess Monitoring: Materials and Devices*	Westin	Westmoreland West-Central
Monday	12:30 PM	178	Topical Plenary: Advances in Biosensing (Invited Talks)	Westin	Pennsylvania West
Monday	3:30 PM	231	Micro and Nanofabricated Sensors	Westin	Pennsylvania West
Tuesday	8:00 AM	265	Biosensors, Bidiagnosis and Bioprocess Monitoring: Cell and Protein Detection*	Westin	Cambria
Tuesday	8:00 AM	279	Electroactive Biomaterials to Sense and Control Microbial Infections*	Westin	Pennsylvania East
Tuesday	8:00 AM	292	Materials Chemistry for Biosensors	Westin	Pennsylvania West
Tuesday	12:30 PM	321	Biosensor Devices: Applications I	Westin	Pennsylvania West
Tuesday	3:30 PM	388	Biosensor Devices: Applications II	Westin	Pennsylvania West

## TA - Immunotherapy

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	454	Enabling Technologies for Immunotherapy Development	Westin	Pennsylvania East
Wednesday	12:30 PM	517	Immunotherapy Applications	Westin	Pennsylvania East
Wednesday	3:30 PM	553	Biomanufacturing	Westin	Pennsylvania East
Thursday	8:00 AM	603	Biomaterials for Immunological Applications*	DLCC	331

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Please refrain from photographing slides or taking video of sessions and presentations.



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# 2018 TECHNICAL PROGRAM GRID

## TB - Food Innovation and Engineering

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	30	Fundamentals of Food, Energy, and Water Systems*	DLCC	320
Sunday	3:30 PM	36	Microbiomes and Metabolomes in Food, Health, and Bioprocessing*	Westin	Westmoreland East
Monday	8:00 AM	57	Advances in Functional Food Production*	Westin	Westmoreland East
Monday	8:00 AM	80	FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)*	DLCC	317
Monday	12:30 PM	151	FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)*	DLCC	317
Monday	3:30 PM	191	Poster Session: Food and Bioprocess Engineering*	DLCC	Exhibit Hall B
Monday	3:30 PM	208	Brewing Education and Training*	DLCC	329
Monday	3:30 PM	246	World Cafe: Food-Energy-Water Nexus (Invited Talks and Panel Discussion)*	DLCC	317
Tuesday	8:00 AM	255	Advances in Membrane Technologies for Food and Bioprocessing*	Westin	Westmoreland East
Tuesday	8:00 AM	304	The Energy-Water Nexus*	DLCC	317
Tuesday	12:30 PM	366	The Food-Energy-Water Nexus*	DLCC	315
Tuesday	3:30 PM	398	Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)*	Westin	Allegheny Grand Ballroom II
Wednesday	8:00 AM	465	Metabolic and Process Engineering for Value-Added Products from Food Processing*	Westin	Westmoreland East

## TC - Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

Day	Time	Session #	Session Title	Property	Room
Tuesday	8:00 AM	283	Environmental Applications of Nanotechnology and Nanomaterials	DLCC	309
Tuesday	12:30 PM	338	Environmental Implications of Nanomaterials: Biological Interactions	DLCC	309
Tuesday	3:30 PM	416	Nanoparticles and Health	DLCC	309

## TD - NH3 Energy+

Day	Time	Session #	Session Title	Property	Room
Wednesday	8:00 AM	434	Ammonia Energy Technology Roadmap	DLCC	318
Wednesday	9:45 AM	485	Ammonia Fuel and Energy Storage: Cracking & Fuel Cells	DLCC	317
Wednesday	9:45 AM	486	Sustainable Ammonia Synthesis: Better & Beyond Haber-Bosch	DLCC	318
Wednesday	1:15 PM	542	Ammonia Combustion: Turbines, Furnaces, Engines	DLCC	317
Wednesday	1:15 PM	543	Sustainable Ammonia Synthesis: Electrochemical Production	DLCC	318
Wednesday	3:30 PM	549	Ammonia Energy Global Demonstrations	DLCC	318
Wednesday	5:30 PM	593	Poster Session: NH3 Energy+ Technologies	DLCC	318

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# 2018 TECHNICAL PROGRAM GRID

## TE - Advances in Fossil Energy R&D

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	11	Advanced Materials for Carbon Dioxide Capture for Power Generation	DLCC	321
Sunday	3:30 PM	46	Reaction Engineering for Combustion and Pyrolysis*	DLCC	402
Monday	8:00 AM	58	Analysis and Design of Carbon Dioxide Capture Technologies for Power Generation	DLCC	321
Monday	8:00 AM	73	Combustion Kinetics and Emissions*	DLCC	402
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	147	Engineering Geologic Carbon Dioxide Storage Systems	DLCC	321
Monday	3:30 PM	187	Poster Session: Advances in Fossil Energy R&D	DLCC	Exhibit Hall B
Monday	3:30 PM	235	Novel Approaches to CO <sub>2</sub> Utilization	DLCC	321
Tuesday	8:00 AM	274	Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems	DLCC	321
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	322	Breakthroughs in C1 to Chemicals and Processing Engineering*	DLCC	318
Tuesday	12:30 PM	370	Value-Added Chemicals from Natural Gas	DLCC	321
Tuesday	3:30 PM	430	Topical Plenary: Advances in Fossil Energy R&D (Invited Talks)	DLCC	321
Wednesday	8:00 AM	439	Advances in Hydrogen and Syngas Production	DLCC	321
Wednesday	12:30 PM	514	Fuel Processing for Hydrogen Production	DLCC	321
Wednesday	3:30 PM	570	Microwave Chemistry for Fuel Conversion	DLCC	321
Thursday	8:00 AM	633	Rare Earth Elements: Extraction, Separation, Characterization, Economics, Criticality, and Kinetics	DLCC	321
Thursday	12:30 PM	646	Application of Solid-Liquid Separation Technologies to Produced Water*	DLCC	301
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols*	DLCC	405
Thursday	12:30 PM	677	New Technologies to Enhance the Production of Unconventional Oil and Natural Gas: Experimentation	DLCC	321
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin*	DLCC	405
Thursday	3:30 PM	713	New Technologies to Enhance the Production of Unconventional Oil and Natural Gas: Simulation	DLCC	321
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry*	DLCC	315
Friday	8:00 AM	733	Modeling and Computation in Energy and Environment*	DLCC	310
Friday	8:00 AM	740	Solid-Fluid Separations in Oil & Gas Production and Refining Processes*	DLCC	303
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks*	DLCC	315

## TG - Innovations of Green Process Engineering for Sustainable Energy and Environment

Day	Time	Session #	Session Title	Property	Room
Sunday	3:30 PM	27	Feedstock Logistics for Biorefineries*	DLCC	316
Sunday	3:30 PM	31	Green Chemical Reaction Engineering for Sustainability*	DLCC	401
Sunday	3:30 PM	41	Novel Catalytic and Separation Process Based on Ionic Liquids	DLCC	318

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# 2018 TECHNICAL PROGRAM GRID

## TG - Innovations of Green Process Engineering for Sustainable Energy and Environment

Day	Time	Session #	Session Title	Property	Room
Monday	8:00 AM	93	Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage	DLCC	318
Monday	8:00 AM	100	Process Research for Improved Throughput & Efficiency, and Reduced Cost & Environmental Impact*	DLCC	335
Monday	11:00 AM	120	The Future of Energy in the Region, Nation and World (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Monday	12:30 PM	144	Efficient Processing of Lignin to Bioproducts and Biofuels I	DLCC	318
Monday	12:30 PM	146	Energy & the Environment U.G. Research Session (Invited Talks)*	DLCC	302
Monday	3:30 PM	216	Efficient Processing of Lignin to Bioproducts and Biofuels II	DLCC	318
Tuesday	8:00 AM	271	Conversion of Solid Wastes to Energy and/or Product	DLCC	319
Tuesday	8:00 AM	306	Topical Plenary: Frontiers in Green Process Engineering (Invited Talks)	DLCC	318
Tuesday	11:00 AM	311	What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)*	DLCC	Spirit of Pittsburgh B
Tuesday	12:30 PM	322	Breakthroughs in C1 to Chemicals and Processing Engineering	DLCC	318
Tuesday	12:30 PM	331	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I*	DLCC	317
Tuesday	12:30 PM	346	Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals*	DLCC	316
Tuesday	12:30 PM	365	Sustainable and Green Product Design*	DLCC	319
Tuesday	3:30 PM	394	Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II*	DLCC	317
Tuesday	3:30 PM	408	Integrated Process Engineering and Economic Analysis	DLCC	318
Wednesday	8:00 AM	462	Ionic Liquids: Thermodynamics and Properties	DLCC	316
Wednesday	3:30 PM	571	Modeling & Simulation of Complex Systems	DLCC	316
Thursday	8:00 AM	613	Distributed Chemical and Energy Processes for Sustainability*	DLCC	317
Thursday	12:30 PM	655	Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols*	DLCC	405
Thursday	3:30 PM	695	Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin*	DLCC	405
Thursday	3:30 PM	726	Value-Added Co-Products from Biorefineries*	DLCC	316
Friday	8:00 AM	730	Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry*	DLCC	315
Friday	12:30 PM	744	Catalytic Upgrading of Alternative Carbon Feedstocks*	DLCC	315

## TJ - WIC 20th Anniversary: Celebrating Women in Chemical Engineering

Day	Time	Session #	Session Title	Property	Room
Tuesday	8:00 AM	309	WIC 20th Anniversary: Celebrating Women in Chemical Engineering I (Invited Talks)	DLCC	Spirit of Pittsburgh A
Tuesday	12:30 PM	371	WIC 20th Anniversary: Celebrating Women in Chemical Engineering II (Invited Talks)	DLCC	Spirit of Pittsburgh A
Tuesday	3:30 PM	432	WIC 20th Anniversary: Celebrating Women in Chemical Engineering III (Invited Talks)	DLCC	Spirit of Pittsburgh A

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**ANSYS: STAY INFORMED - SIMULATION AND ANALYSIS SOFTWARE FOR CHEMICAL AND PROCESS ENGINEERING**  
Wednesday, October 31 • 8:00 AM - 9:15 AM • David L. Lawrence Convention Center, Room 328

Engineering problems and projects are now cross functional and multi-disciplinary. The industry investments are increasingly more complex driven by and for requirements sustainability, energy efficiency, higher performance. Product and process development is also altering by broader adoption of automation tools, digitization trends, and propagation of industrial IoT. Built on a set of well-established physics based modeling and computational techniques engineering simulation has moved from R&D center use to a broader enterprise deployment.

This workshop is designed to highlight the advancements in computational physics tools with focus on material, Chemical, petrochemical, and pharmaceutical industries. Technical examples will include modeling capabilities and applications in reaction and combustion, multiphase, fouling, erosion-corrosion, mixing, separation, battery modeling and more. The content and presentation delivered by industry experts are pulled together to benefit current uses of engineering simulation software (CFD, DEM, FEA, Electromagnetic, System) as well as group leaders, managers, professors, and graduate students interested to learn about the latest advancements in physics based simulation software.



**AVEVA: BENEFITS OF DIGITALIZATION AND AN INTRIGUING USECASE INVOLVING PROCESS SIMULATION**  
Monday, October 29 • 3:30 PM – 4:30 PM • David L. Lawrence Convention Center, Room 326

Much has been written on digitizing the process industries but what is real? This workshop will provide an overview to the benefits and the challenges involved in initiatives such as Industry 4.0 as well as engineering's role in these initiatives. As an example, the use of lifecycle process simulation is explored as a benefit of having a true digital twin of process behavior. Time will be allocated in this workshop for audience feedback on Digital Transformation and how the US compares to Europe in this area.

**AVEVA: GETTING STARTED WITH SIMCENTRAL**

Tuesday, October 30 • 3:30 PM - 5:00 PM • David L. Lawrence Convention Center, Room 301

AVEVA rethinks how process simulation should be done with the release of our next generation process simulation tool, SimCentral. In this 1 ½ hour workshop, we will cover the basics of SimCentral along with its benefits, ease of use and will include a demo and example problems.

Who Should Attend: This workshop is open to all professors, students and members of industry that have interest in process simulation and would like to learn more about SimCentral.

Please stop by our AVEVA/SimSci booth and sign up for a 1-month free license for SimCentral (limited to the first 50 people).



**DIFREX: NEXGEN INNOVATIVE TECHNOLOGY AND SOFTWARE SOLUTIONS, INCLUDING GRM™ GENERAL REACTOR MODEL, FOR EXISTING AND NEW REACTOR SYSTEMS**

Monday, October 29 • 1:45 PM - 3:00 PM • David L. Lawrence Convention Center, Room 326

Wednesday, October 31 • 9:45 AM - 11:00 AM • David L. Lawrence Convention Center, Room 333

Chemical reactors are the most vital elements of the chemical industry, contributing significantly to the total plant cost, efficiency of production, pollution control, number of separation steps needed downstream and therefore to its ultimate profitability.

"Although the reactor is the heart of most process plants, it usually is treated as a 'black box' or a proprietary item and is not covered by commercial simulators. Each technology developer or licensor uses its own procedure to develop its reactor model. Such a procedure often is lengthy and expensive, due to ill-defined steps, many trial-and-error mistakes, and excessive pilot-plant campaigns. Finally, even if the reactor is 'successfully' scaled up to commercial size, the credibility of the design and the optimum operating conditions of the reactor often are questionable." [1]

Come to one of our two Sponsored Technology Workshops and discuss how we can provide the solutions that you need. DIFREX® LLC is a team based in Cape Canaveral, Florida, who provide reactor services and solutions to clients world-wide in areas including design and consulting on existing/new reactor systems, critical review/quick-check of third-party designs, experimental development and validation of proposed designs, debottlenecking/retrofit/revamp, and emergency response.[2]

Let us introduce you to our proprietary state-of-the-art software (including the GRM™), with a comprehensive suite of ready-to-use “design packs” and reactor modules for reactor and reaction modeling. Learn how, as in other cases already handled successfully, we can use the software and our know-how to help you make valid evaluations and select the best Reactor of Choice and Catalyst or Material of Choice at an early stage, generate a Total Solution, and confidently and efficiently progress development and design projects from Concept to Commercialization.

#### References:

[1] Dutta, S. and R. Gualy, “Build Robust Reactor Models”, *Chemical Engineering Progress*, October, 2000, P. 37.

[2] “DIFREX® LLC NEXGEN Reactor Design – Fast assured reactor technology solutions for development, design, optimization, troubleshooting and revamp of commercial reactors” [cited October 29, 2018]; available at [www.difrex.com](http://www.difrex.com).

[3] Dutta, S. and S.C. Arnold, A. Gaurav, J. Brenner, “DIFREX Nexgen Expands and Advances Reactor & Technology Solutions”, *AIChE 2018 Spring Meeting* (April, 2018).

[4] Dutta, S. and S.C. Arnold, A. Gaurav, J. Brenner, “DIFREX Reactor & Technology Solutions for Many Particle Types and Sizes in Catalytic and non-Catalytic Systems”, *8th World Congress on Particle Technology* (April, 2018).



### **INNOVATIA: BRIDGING THE GAP BETWEEN ENGINEERING AND OPERATIONS: WORK AS DESIGNED VS. WORK AS PERFORMED**

**Tuesday, October 30 • 3:30 PM - 4:45 PM • David L. Lawrence Convention Center, Room 332**

Each day work is executed by people within dangerous and complex processes using equipment that was designed to operate in a highly specific way. A persistent challenge is reconciling work as designed vs. work as performed. A lot of research has gone into solving this problem and the human element is often at the center of the conversation. The paper “Why major accidents are still occurring<sup>1</sup>” suggests that human error, management focus, culture and knowledge management and communication are the gaps in the equation today.

Strides have been made over the years in safety programs, HSSE initiatives, management oversight, regulatory requirements, culture shift and education. An emerging opportunity exists in journey towards a “goal zero” incident. It is the explosion of digital technology capable of giving front line employees the knowledge they need to execute work, properly, every time. During this session, we will explore opportunities to align work as designed vs. work as executed using the latest in knowledge management and communication technologies.

<sup>1</sup> Paul R Amyotte, Scott Berger, David, W Edwards, Jai P Gupta, Dennis C Hendershot, Faisal I Khan, M Sam Mannan, and Ronald J Willey

### **INNOVATIA: THE DIGITAL WORKPLACE AT THE FRONT LINE AND WHERE TO BEGIN: BEYOND THE DIGITAL TWIN**

**Wednesday, October 31 • 3:30 PM - 4:45 PM • David L. Lawrence Convention Center, Room 336**

The first step for the workplace digitization would be the creation of a Digital Twin of your plants. Digital Twin is a digital replica of your physical assets, and it is used for various purposes integrating artificial intelligence, machine learning, and software analytics to create digital simulation models that are updated as their physical counterparts’ change. One important note, do not forget to add human factors to this equation.

That is when things start to get tricky, because unlike the machines, people are unpredictable and subject to error. The challenge ahead of us is to increase the predictability by which people work – close the gap between work as designed vs. work as executed. Digitized knowledge management systems will set the foundation to deliver the right information where and when it is needed. The connected worker of tomorrow can execute work in a more standardized way while collecting data, similar to the way IIOT sensors collect data today on equipment.

The beauty of it is that it can be done with the user experience in mind to allow humans to excel at what humans are good at, solving problems, creating value and contributing to improvement. The fundamentals of the various frameworks for process improvement rely on capturing knowledge from the front lines. This can be made ever more effective using today's information and communication technology to have operators take ownership of the whole process while operating as designed.



### **KNOVEL: DRIVING DIGITAL TRANSFORMATION IN CHEMISTRY & ADVANCED MATERIALS INDUSTRY THROUGH DECISION SUPPORT INFORMATION SOLUTIONS WITH AN OVERVIEW OF AIChE'S KNOVEL SUBSCRIPTION**

**Monday, October 29 • 4:45 PM - 6:00 PM • David L. Lawrence Convention Center, Room 328**

Chemistry and Advanced Materials industry is expected to follow a rather evolutionary approach to digitalization. Based on a recent report by the World Economic Forum, three themes are expected to underpin the digital transformation - Digitalize the Enterprise; Go Beyond the Molecule; Collaborate in Ecosystems. Talk will touch upon how Elsevier is helping drive digital transformation through a Decision Support Solution, bringing together relevant scientific, commercial & company data in one place for chemists/engineers/Tox/safety/regulatory professionals to help reduce risk & collaborate, driving innovation & faster products to market. This presentation will also highlight the Knovel subscription that is a member benefit for AIChE members highlighting recent features added to the application.



## **PROCESS SYSTEMS ENTERPRISE: HANDS-ON WORKSHOP - DIGITAL DESIGN OF ROBUST FORMULATED PRODUCTS AND THEIR MANUFACTURING PROCESSES THROUGH MECHANISTIC MODELLING**

**Wednesday, October 31 - 8:00 AM - 10:30 AM • The Westin, Washington Room**

Join PSE and industry experts for a hands-on experience with gPROMS FormulatedProducts, an innovative platform for the digital design of formulated products and their manufacturing processes. Scientists and engineers in the pharmaceutical, biopharmaceutical, food and consumer goods industries face challenges in efficiently bringing products to market with robust manufacturing processes to produce the desired end-use attributes. gPROMS FormulatedProducts allows scientists and engineers to screen formulations for end-user attributes, determine whether they can be manufactured efficiently and robustly, and explore the design space of the whole formulation and manufacturing chain.

In this workshop, attendees will choose from a variety of hands-on modules that demonstrate model configuration, validation with experimental data, optimization, and sensitivity analysis for a particular application. Application areas include:

- Synthesis and fluid separation,
- Crystallization,
- Wet milling,
- Spray drying,
- Continuous direct compression,
- Wet and dry granulation,
- Oral absorption, and
- End-to-end modeling (e.g. putting Systems-based Pharmaceutics into practice).

## **PROCESS SYSTEMS ENTERPRISE: INTRODUCTION TO PROCESSBUILDER - HOW TO CREATE VALUE FOR YOUR RESEARCH AND BUSINESS**

**Wednesday, October 31 - 3:30 PM - 6:00 PM • David L. Lawrence Convention Center, Room 320**

Join PSE and industry experts for a workshop on gPROMS ProcessBuilder, a next-generation Advanced Process Modeling environment for optimizing the design and operation of process plants. gPROMS ProcessBuilder combines industry-leading steady-state and dynamic models with all the power of equation-oriented modeling, system analysis and optimization in an easy-to-use process flowsheeting environment. Its predictive power enables scientists and engineers to scale up their pilot plants in a more efficient manner, explore the process design and operational space rapidly and make better, faster and safer decisions. Models can be used in on-line applications and can be deployed behind a web interface in just a couple of hours.

This workshop will show how gPROMS ProcessBuilder is transforming the way the process industries are unlocking new value and competitive advantage. Illustration of key features with application examples and hands-on exercises include:

- Robust solution of a process flowsheet with complex recycles
- Detailed first-principles model integrated within a flowsheet
- Custom modeling
- Global system analysis
- Model validation
- Whole plant optimization including mixed-integer optimization
- Web deployment & on-line use

## **Rockwell Automation**

### **ROCKWELL AUTOMATION: PROCESS SAFETY – THE LIFECYCLE EXPLAINED**

**Monday, October 29 • 12:30 PM – 1:45 PM • David L. Lawrence Convention Center, Room 332**

The Process Safety lifecycle has been around for over 20 years, this workshop explains the history, what we have learned in the industry, how the standards have evolved and how we use the lifecycle approach to minimize risk and optimize production.

## **SIEMENS**

*Ingenuity for life*

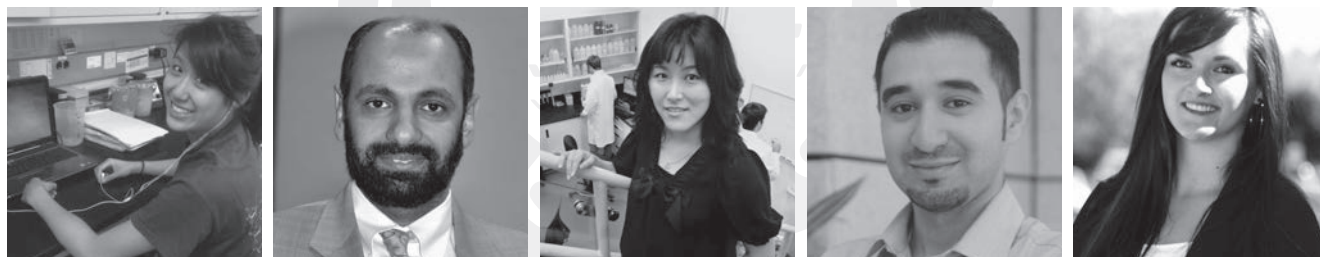
### **SIEMENS PLM SOFTWARE: ADVANCED SIMULATION (CFD & DEM) TO SOLVE CHALLENGES IN THE PROCESS INDUSTRY**

**Wednesday, October 31 • 12:30 PM - 3:00 PM • David L. Lawrence Convention Center, Room 336**

Understanding of transport processes (fluid flow, heat transfer & mass transfer) is key for design, troubleshooting and exploring optimum operating conditions. In this workshop we will look at two most important aspects of the problems encountered: turbulence and multiphase flow phenomenon. Computational fluid dynamics (CFD) and particle modeling with Discrete Element Method (DEM) have been identified as key enabling technologies in finding solutions to many of the challenges that surround scale-up; capable of reducing operating costs across manufacturing and quality divisions. We will then use this basis to show examples of how this can be used to solve problems as well as demonstrate the use of Simcenter STAR-CCM+, a multiphysics simulation platform from Siemens. All presenters will be available to answer questions.



# It's Never Been Easier to Get Engaged with AIChE® Members.



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## Find Opportunities to Get Involved on Volunteer Central

AIChE now offers volunteer opportunities to help you give back to the Chemical Engineering community. Fill out your volunteer profile to see volunteer opportunities tailored to your interests, or you can browse all AIChE volunteer opportunities.





# Secure Your Spot and Mark Your Calendar for These **AIChE®** Events.



## Biological and Metabolic Engineering

### International Conference on Microbiome Engineering

November 4-6, 2018  
Boston, MA

### 2nd International Conference on Plant Synthetic Biology, Bioengineering, and Biotechnology

November 29-December 1, 2018  
Clearwater, FL

### 6th International Conference on Stem Cell Engineering 2018

December 5-7, 2018  
Los Angeles, CA

### 2nd International Conference on CRISPR Technologies

December 10-12, 2018  
San Diego, CA

### 3rd Symposium on Complex Biodynamics & Networks

December 10-12, 2018  
Biopolis, Singapore

### 9th ICBE—International Conference on Biomolecular Engineering

January 6-9, 2019  
Newport Beach, CA

### 2nd Rock Stars of Regenerative Engineering

January 9, 2019  
San Francisco, CA

### 6th International Conference on Accelerating Biopharmaceutical Development (AccBio 2019)

February 17-19, 2019  
Carlsbad, CA

### Commercializing Industrial Biotechnology 2019

May 13-14, 2019  
Los Angeles, CA

### 8th International Conference on Bioengineering and Nanotechnology

May 28-31, 2019  
Baltimore, MD

### 2019 Synthetic Biology: Engineering, Evolution & Design (SEED)

June 23-27, 2019  
New York, NY



## Chemical Engineering Practice

### Space Travel: Adaptive Research and Technologies from Biological and Chemical Engineering (STAR Tech)

November 12-14, 2018  
Houston, TX

### Food Innovation and Engineering (FOODIE) Conference

December 2-4, 2018  
Napa, CA

### 3rd Ethylene Middle East Technology Conference and Exhibition (EMET)

December 11-12, 2018  
Kingdom of Bahrain

### Council for Chemical Research Annual Meeting

December 17-18, 2018  
Wilmington, DE

### 2019 AIChE Spring Meeting and 15th Global Congress on Process Safety

March 31- April 4, 2019  
New Orleans, LA

### International Congress on Particle Technology

April 9-11 2019  
Nürnberg, Germany

### Chemical Ventures Conference 2019

April 23-24, 2019  
Wilmington, DE

### North American Membrane Society (NAMS) 2019 Annual Meeting

May 11-15, 2019  
Pittsburgh, PA

### Fluidization XVI

May 26-31, 2019  
Guilin, China

### Summer Heat Transfer Conference (SHTC)

July 15-18, 2019  
Bellevue, WA

### 2019 AIChE Annual Meeting

November 10-15, 2019  
Orlando, FL

### 2020 AIChE Spring Meeting and 16th Global Congress on Process Safety

March 29-April 2, 2020  
Houston, TX



## Energy

### Arctic Technology Conference

November 5-7, 2018  
Houston, TX

### Offshore Technology Conference

May 6-9, 2019  
Houston, TX

### 14th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering (GLS-14)

May 30-June 3, 2019  
Guilin, China

### 12th Natural Gas Conversion Symposium New Vistas on Shale

June 2-6, 2019  
San Antonio, TX



## Process Safety

### 2018 European Conference on Process Safety and Big Data

November 14-15, 2018  
Frankfurt am Main, Germany

### 2019 AIChE Spring Meeting and 15th Global Congress on Process Safety

March 31-April 3, 2019  
New Orleans, LA

### 64th Annual Safety in Ammonia Plants and Related Facilities Symposium

September 8-12, 2019  
San Francisco, CA



## Sustainability and Environment

### Technical and Engineering Challenges of Addressing the United Nations Sustainable Development Goals

November 1-2, 2018  
Pittsburgh, PA

### Industrial Water Use and Reuse Workshop 2018

November 15-16, 2018  
San Antonio, TX

### 2019 Carbon Management Technology Conference

July 15-18, 2019  
Houston, TX



# 2018 AIChE INSTITUTE/BOARD AWARDS + MAJOR LECTURES

SUNDAY, OCTOBER 28

## HONORS CEREMONY

5:15 PM – 6:45 PM • David L. Lawrence Convention Center, Spirit of Pittsburgh Ballroom B

Join your colleagues in honoring the recipients of the 2018 Board of Directors' and Institute Awards.

## BOARD OF DIRECTORS' AWARD RECIPIENTS



**Founders Award for Outstanding Contributions to the Field of Chemical Engineering**

**Julio M. Ottino**  
Dean, *Northwestern University*



**F. J. and Dorothy Van Antwerpen Award for Service to the Institute**

(Award sponsored by The Dow Chemical Company)

**Eduardo D. Glandt**  
Nemirovsky Family Dean Emeritus  
*University of Pennsylvania*

## INSTITUTE AWARD RECIPIENTS



**Allan P. Colburn Award for Excellence in Publications by a Young Member of the Institute**

(Award sponsored by E. I. DuPont de Nemours & Company)

**Hal S. Alper**  
Professor, *University of Texas at Austin*



**Alpha Chi Sigma Award for Chemical Engineering Research**

(Award sponsored by the Alpha Chi Sigma Fraternity & the Alpha Chi Sigma Educational Foundation)

**Eric S. G. Shaqfeh**  
Professor, *Stanford University*



**Andreas Acrivos Award for Professional Progress in Chemical Engineering**

(Award endowed by The AIChE Foundation)

**Martin Z. Bazant**  
E. G. Roos (1944) Professor,  
*Massachusetts Institute of Technology*



**Industry Leadership Award**

**Jean W. Tom**  
Head, Development Engineering  
*Bristol-Myers Squibb*



**Industrial Research and Development Award**

**Kristin Thunhorst**  
Scientist, *3M*



**Industrial Progress Award**

**Michael D. Determan**  
Senior Technical Manager, *3M*

## INSTITUTE AWARD RECIPIENTS (continued)


**Institute Award for Excellence in Industrial Gases Technology**

(Award sponsored by Praxair, Inc.)

**David Sholl**

John F. Brock III School Chair  
*Georgia Institute of Technology*


**Institute Award for Service to Society**
**Daniel J. Lacks**

C. Benson Branch Professor  
*Case Western Reserve University*


**Lawrence B. Evans Award in Chemical Engineering Practice**

(Award endowed by The AIChE Foundation with support from CACHE Corporation)

**Ronald R. Chance**

Vice President, Engineering  
*Algenol Biotech LLC*


**Margaret Hutchinson Rousseau Pioneer Award for Lifetime Achievement by a Woman Chemical Engineer**

(Award sponsored by Pfizer)

**Elsa Reichmanis**

Professor and Peter Silas Chair  
*Georgia Institute of Technology*


**R. H. Wilhelm Award in Chemical Reaction Engineering**

(Award sponsored by The ExxonMobil Research and Engineering Company)

**Linda J. Broadbelt**

Sarah Rebecca Roland Professor and Associate Dean for Research  
*Northwestern University*


**Warren K. Lewis Award for Chemical Engineering Education**

(Award sponsored by The ExxonMobil Research and Engineering Company)

**Babatunde A. Ogunnaike**

Dean, College of Engineering  
*University of Delaware*


**William H. Walker Award for Contributions to Chemical Engineering Literature**

(Award sponsored John Wiley and Sons)

**Enrique Iglesia**

Professor, *University of California, Berkeley*

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## FEATURED LECTURES



### 2018 DANCKWERTS LECTURE

Monday, October 29 • 11:15 AM – 12:15 PM

The Westin Convention Center, Allegheny Ballroom II

#### Biotechnology to Help Achieve the UN's Sustainable Development Goals

Sang Yup Lee, Distinguished Professor of Chemical and Biomolecular Engineering

*Korea Advanced Institute of Science and Technology*



### D.I.C. WANG AWARD LECTURE

Monday, October 29 • 6:00 PM – 7:00 PM

The Westin Convention Center, Allegheny Ballroom I

#### Lessons from a Life in Biopharma

John G. Auniņš, Executive Vice President and Chief Technology Officer, *Seres Therapeutics, Inc.*



### 2018 ANDREAS ACRIVOS AWARD FOR PROFESSIONAL PROGRESS IN CHEMICAL ENGINEERING LECTURE

Tuesday, October 30 • 11:15 AM – 12:15 PM

David L. Lawrence Convention Center, Spirit of Pittsburgh Ballroom A

#### Microscale Engineering of Responsive, Flexible and Reconfigurable Particle Structures

Orlin D. Velev, INVISTA Professor, *North Carolina State University*



### SBE'S JAMES E. BAILEY AWARD LECTURE

Tuesday, October 30 • 6:00 PM – 7:00 PM

The Westin Convention Center, Allegheny Ballroom I

#### Turning Immunity On and Off

Jeffrey A. Hubbell, Eugene Bell Professor in Tissue Engineering, Institute for Molecular Engineering

*University of Chicago*



### AWARD PRESENTATION

Biotechnology Progress Award for Excellence in Biological Engineering Publication

Junghae Suh, Associate Professor, *Rice University*



### JOHN M. PRAUSNITZ AIChE INSTITUTE LECTURE

Wednesday, October 31 • 11:15 AM – 12:15 PM

David L. Lawrence Convention Center, Spirit of Pittsburgh Ballroom A

#### Accelerating Development and Intensification of Chemical Processes

Klavs F. Jensen, Warren K. Lewis Professor of Chemical Engineering and Professor of Materials Science and Engineering, *Massachusetts Institute of Technology*

## FEATURED SESSIONS

### THE FUTURE OF ENERGY IN THE REGION, NATION AND WORLD ■

Monday, October 29 • 11:00 AM – 12:30 PM

David L. Lawrence Convention Center, Spirit of Pittsburgh Ballroom B

#### PANELISTS



**Bruce Garrett**

Division Director, Chemical Sciences, Geosciences, and Biosciences, Basic Energy Sciences, Office of Science, U.S. Department of Energy



**Kamel Ben-Naceur**

Chief Economist, *ADNOC*



**TJ Wojnar**

Vice President of Corporate Strategic Planning, *Exxon Mobil Corporation*



#### MODERATOR

**J. Karl Johnson**

W. K. Whiteford Professor  
Department of Chemical & Petroleum Engineering  
Associate Director, Center for Simulation & Modeling  
*University of Pittsburgh*

### WHAT THE HECK HAPPENED? PAST, PRESENT & FUTURE DISRUPTIONS TO THE CHEMICALS/FUELS BUSINESS ■

Tuesday, October 30 • 11:00 AM – 1:30 PM

David L. Lawrence Convention Center, Spirit of Pittsburgh Ballroom B

#### PANELISTS



**Scott Mitchell**

Global Catalysis Leader, Innovation and Technology, *Braskem*



**Antonis Papadourakis**

President and CEO, *LANXESS Corporation*



**Joseph Powell**

Chief Scientist - Chemical Engineering, *Shell*



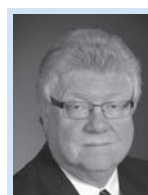
**Jeffrey Sirola**

Professor of Engineering Practice  
*Purdue University & Carnegie Mellon University*



**David West**

Corporate Fellow and Director of Corporate Research and Innovation  
*SABIC*



#### MODERATOR

**Cliff Kowall**

Senior Technical Fellow – Corporate Engineer  
Process Innovation & University Collaboration  
*The Lubrizol Corporation (Berkshire Hathaway)*  
Adjunct Faculty Member  
Department of Chemical & Petroleum Engineering  
*University of Pittsburgh*

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## FEATURED SESSIONS

### AIChE's 110 YEAR CELEBRATION

Tuesday, October 30 • 3:30 PM – 6:00 PM  
David L. Lawrence Convention Center, 303



### SPEAKERS



#### **25 by 25: Chemical Engineering in the Next 25 Years**

##### **Clare McCabe**

Cornelius Vanderbilt Professor of Engineering, Associate Dean for Postdoctoral Affairs, and Director, VINSE Research Experience for Undergraduates  
*Vanderbilt University*



#### **The Future of Chemical Engineering Itself**

##### **Phil Westmoreland**

Professor of Chemical and Biomolecular Engineering, *North Carolina State University*  
Executive Director  
*NCSU Institute for Computational Science and Engineering*



#### **Accelerating Innovation through Academic-Industrial Partnerships**

##### **Bill Liechty**

Associate Research Scientist  
*The Dow Chemical Company*



#### **Maximizing Uptime, Efficiency, and Safety of Industrial Operations through Early Risk Detection**

##### **Ankur Pariyani**

Co-Founder/Chief Innovation Officer  
*Near-Miss Management LLC*



#### **Gaussian Processes for Hybridising Analytical and Data-driven Decision-making**

##### **Ruth Misener**

Lecturer and Assistant Professor  
*Imperial College London*



### **MODERATOR**

##### **Lorenz T. Biegler**

Covestro University Professor and Head, Chemical Engineering Department  
*Carnegie Mellon University*

# SAVE THE DATE

NOVEMBER 10-15, 2019 • HYATT REGENCY, ORLANDO, FLORIDA

## HIGHLIGHTS WILL INCLUDE:

- “Meet the Innovators” featured session on Monday, November 11
  - Programming from AIChE's technical divisions and forums
- Brand new topical conferences highlighting the latest research and technology
  - Innovative poster receptions
  - Much more!



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# YOUNG PROFESSIONAL AND GRADUATE STUDENT SESSIONS & EVENTS

Recommended by the AIChE® Young Professionals Committee

## SUNDAY, OCTOBER 28

**Workshop: Career Planning for Prospective Faculty** • David L. Lawrence Convention Center • 10:00 AM - 12:00 PM • ROOM: 408

**Primary Sponsor:** Professional Development Committee Liaison • **Co-Sponsor:** Young Professionals Committee (YPC)

**Chemical Engineering in Sustainability (YCOSST) and Policy (WISE) Award Recipient Talks (Invited Talks)**

David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 307

**Primary Sponsor:** Young Professionals Committee (YPC)

**Co-Sponsor:** The Food-Energy-Water Nexus; International Congress on Energy (ICE) 2018

**Panel Discussion: Chemical Process and Product Design Careers** • David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 326

**Primary Sponsor:** Product Design • **Co-Sponsor:** Young Professionals Committee (YPC)

**Workshop: Effective Teaching for New or Prospective Faculty** • David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 411

**Primary Sponsor:** Undergraduate Education • **Co-Sponsor:** Young Professionals Committee (YPC)

**Young Professionals Social (\$10 cash only)** • Sienna Mercato, 942 Penn Ave (1 block from Convention Center)

## MONDAY, OCTOBER 29

**Managing and Leading Teams & Running an Effective Meeting - TICKETED EVENT** • David L. Lawrence Convention Center

8:00 AM - 11:00 AM • ROOM: 326

**Advanced Problem Solving in the Chemical Industry I** • David L. Lawrence Convention Center • 12:30 PM - 3:00 PM • ROOM: 407

**Primary Sponsor:** Young Professionals Committee (YPC)

**Energy & the Environment U.G. Research Session (Invited Talks)** • David L. Lawrence Convention Center

12:30 PM - 3:00 PM • ROOM: 302

**Primary Sponsor:** Young Professionals Committee (YPC)

**Co-Sponsor:** Innovations of Green Process Engineering for Sustainable Energy and Environment; Sustainable Energy

**Experiences in Teaching Process Safety** • David L. Lawrence Convention Center • 12:30 PM - 3:00 PM • ROOM: 335

**Primary Sponsor:** Product Design • **Co-Sponsor:** Young Professionals Committee (YPC)

**Managing Yourself: Reinventing Yourself for Your Next Role** • David L. Lawrence Convention Center • 12:30 PM - 3:00 PM • ROOM: 331

**Primary Sponsor:** Management Division • **Co-Sponsor:** Young Professionals Committee (YPC)

**Brewing Education and Training** • David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 329

**Sponsor:** TB Food Innovation and Engineering

**Advanced Problem Solving in the Chemical Industry II** • David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 407

**Primary Sponsor:** Young Professionals Committee (YPC)

**Green Chemistry and Engineering** • David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 309

**Primary Sponsor:** General • **Co-Sponsor:** Young Professionals Committee (YPC)

**Networking for Nerds: How to Create Your Dream Career** • David L. Lawrence Convention Center • 3:30 PM - 4:40 PM • ROOM: 330

**Primary Sponsor:** Publication Committee • **Co-Sponsor:** Young Professionals Committee (YPC)

**MONDAY, OCTOBER 29 (continued)**

**Young Professionals Committee Meeting (All welcomed)** • Westin Hotel, Butler • 4:00 PM - 5:30 PM

**Young Professional Research Projects in Industry (Invited Talks)** • David L. Lawrence Convention Center • 8:00 AM - 10:30 AM • ROOM: 303

**Primary Sponsor:** Young Professionals Committee (YPC)

**Co-Sponsor:** Research and New Technology Committee (RANTC); Process Research and Innovation; Technology Transfer and Manufacturing

**Biotechnology & Materials U.G. Research Session (Invited Talks)** • David L. Lawrence Convention Center • 8:00 AM - 10:30 AM • ROOM: 302

**Primary Sponsor:** Young Professionals Committee (YPC) • **Co-Sponsor:** Bionanotechnology

**Design, Construction, and Operation of Unit Operations Labs and Pilot Plants** • David L. Lawrence Convention Center  
8:00 AM - 10:30 AM • ROOM: 336

**Primary Sponsor:** Pilot Plants • **Co-Sponsor:** Young Professionals Committee (YPC)

**Using the Brains of Others to Innovate Faster** • David L. Lawrence Convention Center • 8:00 AM - 10:30 AM • ROOM: 331

**Primary Sponsor:** Professional Development • **Co-Sponsor:** Young Professionals Committee (YPC)

**Marketing is Not Bragging: How to Articulate Your Value to Advance Your Career** • David L. Lawrence Convention Center  
4:45 PM - 6:00 PM • ROOM: 330

**Primary Sponsor:** Publication Committee • **Co-Sponsor:** Young Professionals Committee (YPC)

**TUESDAY, OCTOBER 30**

**Advanced Problem Solving in the Chemical Industry III** • David L. Lawrence Convention Center • 8:00 AM - 10:30 AM • ROOM: 407

**Primary Sponsor:** Young Professionals Committee (YPC)

**Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects** • David L. Lawrence Convention Center  
8:00 AM - 10:30 AM • ROOM: 331

**Primary Sponsor:** Management Division • **Co-Sponsor:** Young Professionals Committee (YPC)

**Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)** • David L. Lawrence Convention Center  
8:00 AM - 10:30 AM • ROOM: 306

**Primary Sponsor:** Electrochemical Fundamentals • **Co-Sponsor:** Young Professionals Committee (YPC)

**Young Faculty Forum (Invited Talks)** • David L. Lawrence Convention Center • 8:00 AM - 10:30 AM • ROOM: 407

**Primary Sponsor:** Young Faculty Forum • **Co-Sponsor:** Young Professionals Committee (YPC)

**Advanced Problem Solving in the Chemical Industry IV** • David L. Lawrence Convention Center • 12:30 PM - 3:00 PM • ROOM: 407

**Primary Sponsor:** Young Professionals Committee (YPC)

**Management Award and Executive Leadership Topics** • David L. Lawrence Convention Center • 12:30 PM - 3:00 PM • ROOM: 331

**Primary Sponsor:** Management Division • **Co-Sponsor:** Young Professionals Committee (YPC)

**AIChE's 110 Year Celebration (Invited Talks)** • David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 303

**Primary Sponsor:** Miscellaneous • **Co-Sponsor:** Young Professionals Committee (YPC)

**Applied Project Management Fundamentals: A Tutorial** • David L. Lawrence Convention Center • 3:30 PM - 6:00 PM • ROOM: 331

**Primary Sponsor:** Management Division • **Co-Sponsor:** Young Professionals Committee (YPC)



For more information on each session, please use the Conference App.



DIVERSITY &  
INCLUSION

# AICHE

The Global Home of Chemical Engineers



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Attend one or all of the many events and sessions focusing on the  
positive societal impact made by chemical engineers  
**#allforgood**

## Chemical Engineers Impacting Society Events

You're invited to attend the following events advancing Diversity & Inclusion and showcasing chemical engineers' contributions to our global society.

### Sunday, October 28

#### Women's Initiatives Committee (WIC) Developing your Career for Women Graduate Students and Beyond (Ticketed Event)

9:00 AM – 1:30 PM

David L. Lawrence Convention Center, 316

#### Women's Initiatives Committee (WIC) Women Undergraduates Workshop (Ticketed Event)

9:00 AM – 12:00 PM

David L. Lawrence Convention Center, 315

#### Minority Affairs Committee (MAC) MAC Real Talk: Speed Mentoring for Undergraduates (Ticketed Event)

9:30 AM – 12:30 PM

Westin Convention Center

Allegheny II

#### ChemE's with Disabilities + Allies - Expanding Opportunities and Creating Community

2:00 PM – 3:00 PM

Westin Convention Center

Pennsylvania East

#### ChemE's with Disabilities + Allies Reception/Forum

5:30 PM – 6:30 PM

David L. Lawrence Convention Center, 312

### Monday, October 29

#### Diversity and Inclusion: Cultural Competency Workshop

8:30 AM – 10:30 AM

David L. Lawrence Convention Center, 315

#### Women's Initiatives Committee Luncheon (WIC) (Ticketed Event)

11:00 AM – 12:30 PM

Westin Convention Center

Allegheny Grand Ballroom III

#### Minority Affairs Committee (MAC) MAC Planning Workshop

12:30 PM – 2:30 PM

David L. Lawrence Convention Center, 304

#### Minority Affairs Committee (MAC) MAC Eminent Engineers Awards Ceremony

5:30 PM – 7:00 PM

David L. Lawrence Convention Center, 325

#### Minority Affairs Committee (MAC) MAC Reception

7:00 PM – 9:00 PM

David L. Lawrence Convention Center, 324

### Tuesday, October 30

#### WIC 20th Anniversary Symposium: Celebrating Women in Chemical Engineering: Invited Talks

8:00 AM – 6:00 PM

Spirit of Pittsburgh Ballroom A

#### Minority Affairs Committee (MAC) MAC/MFF Real Talk: Navigating the Academic Career Path to Tenure (Ticketed Event)

11:00 AM – 12:30 PM

Westin Convention Center

Allegheny Grand Ballroom III

#### ChemE's with Disabilities + Allies Practical Adaptations for Teaching Students with Disabilities

1:45 PM – 2:10 PM

David L. Lawrence Convention Center, 411

#### LGBTQ + Allies Inclusion Workshop/Panel

3:30 PM – 6:00 PM

David L. Lawrence Convention Center, 407

#### LGBTQ+ Allies Reception: Hosted by AIChE Leadership

6:00 PM – 7:15 PM

Westin Convention Center

Cambria, 2nd Floor

# 2018 TECHNICAL SESSIONS

## (1) Workshop: Hands On With Molecular Simulation (Ticketed Event)

Sunday, Oct 28, 8:00 AM

David L. Lawrence Convention Center, 334

Eric Jankowski, Chair  
Sapna Sarupria, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**8:00 Paper 1a:** MoSDeF: Molecular Simulation and Design Framework — **Peter T. Cummings**

**9:10 Paper 1b:** Advanced Sampling Using Ssages: Basics, Practical Tips and More — **Jonathan K. Whitmer**

**10:20 Paper 1c:** Design Problems with Biomolecules — **Heather Mayes**

**11:30 Paper 1d:** GOMC: GPU Optimized Monte Carlo — **Jeffrey J. Potoff**

**12:40 Paper 1e:** Managing Data Spaces, Performing MD, and Analyzing Trajectories with Signac, HOOMD-Blue, and Freud — **Carl Simon Adorf, Vyas Ramasubramani, Joshua A. Anderson, Sharon C. Glotzer**

**1:50 Paper 1f:** Physically Validating Molecular Simulation Results — **Michael Shirts**

## (2) Women Undergraduates Workshop (Ticketed Event)

Sunday, Oct 28, 9:00 AM

David L. Lawrence Convention Center, 315

Shannon L. Servoss, Chair  
Bindu Krishnan, Co-Chair

**Sponsored by:** Women's Initiatives Committee (WIC)

## (3) Developing Your Career for Women Graduate Students and Beyond (Ticketed Event)

Sunday, Oct 28, 9:00 AM

David L. Lawrence Convention Center, 316

Shannon L. Servoss, Chair  
Bindu Krishnan, Co-Chair

**Sponsored by:** Women's Initiatives Committee (WIC)

## (4) Workshop: Career Planning for Prospective Faculty

Sunday, Oct 28, 10:00 AM

David L. Lawrence Convention Center, 408

Timothy Anderson, Chair

**Sponsored by:** Professional Development Committee Liaison

**10:00 Paper 4a:** Presentation and Workshop on Career Planning — **Timothy Anderson, Geoffrey A. Prentice**

## (5) Chem-E-Car Competition

Sunday, Oct 28, 12:30 PM

David L. Lawrence Convention Center, Exhibit Hall C

Sarah Ewing, Chair

**Sponsored by:** Student Chapters Committee Liaison

## (6) Meet the Faculty Candidate Poster Session

Sunday, Oct 28, 1:00 PM

David L. Lawrence Convention Center, Exhibit Hall B

Sundararajan V. Madhally, Chair  
Roman Voronov, Co-Chair

**Sponsored by:** Meet the Faculty Candidate Poster Session – Sponsored by the Education Division

## ■ BIOMATERIALS & BIOLOGICAL ENGINEERING

**Paper 6a:** Molecular Machines As Tools for Engineering with Biological Systems — **Kyle E. Watters**

**Paper 6b:** Functional Biomaterials for Smart Delivery of Therapeutics — **Lisa R. Volpatti**

**Paper 6c:** Molecular Recognition: From Polymer Science to Precision Medicine — **John R. Clegg**

**Paper 6d:** Morphological Aspects in Materials for Biotechnological Applications — **Jyothirmai J. Simhadri**

**Paper 6e:** Microfluidic Bioanalytical Systems: From Point of Care Detection of Infectious Agents to Analysis of Biomarkers on Mars — **Thomas N. Chiesl**

**Paper 6g:** Transformation of Waste Biomass into Bioproducts (Bioenergy, Biomaterials, Biochemicals) — **Ezinne Achinivu**

**Paper 6h:** Bio-Inspired, Self-Organizing Soft Materials — **Kimberly L. Weirich**

**Paper 6i:** Application of Ultrasound for Synthesis of Carbon Capture Microcapsules — **Srinivas Mettu**

**Paper 6j:** Evaluation on the Removal Performance of Dichloromethane and Toluene from Waste Gases Using a Novel Airflow Packing Reactor — **Peilun Xu, Xiang-Qian Wang, Su-Jing Li, Wei Li**

**Paper 6k:** Leveraging Mechanistic Understanding of Triacylglycerides and Astaxanthin in Supercritical Carbon Dioxide for Selective Separation Processes from Microalgae — **Thomas Kwan**

**Paper 6l:** Rational Fabrication of Biomaterial-Based Scaffolds, Devices and Films for Tissue Engineering, Drug/Gene Delivery, Biomedical Processes and Flexible Electronics — **Metin Uz**

**Paper 6m:** Biomolecular Engineering and Ultrasound-Enhanced Transport in Neuroscience — **Jerzy O. Szablowski**

**Paper 6n:** Protein Engineering for Cell- and Ligand-Based Immunotherapy — **Lawrence A. Stern**

**Paper 6o:** Life Science Systems Engineering — **Maria M. Papathanasiou**

**Paper 6p:** Optical Imaging of the Brain at Nanoscopic Resolution — **Ruixuan Gao, Edward S. Boyden**

**Paper 6q:** Engineering Protein Specificity: New Tools and Biologics to Remediate Human Diseases — **Carl A. Denard, Brent L. Iverson**

**Paper 6r:** Engineering 3D Models of Cancer through Application of Biomaterials and Systems Biology — **Kaitlin Fogg**

**Paper 6s:** Integrated Gene Circuit Design and Cellular Engineering: Probing and Reshaping the Genome to Control Cell Fate — **Kate E. Galloway**

**Paper 6u:** Imitating Nature's Approach: Molecular Engineering of Organic Materials for Energy and Sensing — **Suchol Savagatrup**

**Paper 6v:** Advancing Technologies for Protein Engineering, Metabolic Engineering, and High-Throughput Technologies — **Jyun-Liang Lin**

**Paper 6w:** New Routes Toward Biomass-Derived Carbohydrates Upgrading — **Ydna M. Questell-Santiago**

**Paper 6x:** Engineering Multienzyme Systems for the Next Generation of Biomanufacturing — **Yifei Zhang**

**Paper 6y:** Unifying Engineering and Synthesis to Create Platform Biomaterials — **Owen S. Fenton, Robert Langer**

**Paper 6z:** On-Demand Therapeutics: From Externally-Triggerable Drug Delivery Systems to Bioelectronics — **Alina Rwei**

**Paper 6aa:** Stability of Recombinant Protein-Based Bio-Pharmaceuticals: Stability in the Glassy Lyophilized State, at Various Interfaces and in Bulk Bio-Manufacturing Flows — **Jai A. Pathak**

**Paper 6ab:** Multiscale Multiphysics Modeling of Blood Clotting and Thrombus Bio-Chemomechanics in the Vasculature — **Alireza Yazdani**

**Paper 6ac:** Preparing of a Composite Nano Disperse Dye Using a Hydroxypropyl Sulfonated Lignin Dispersant and the Interaction of Dispersant and Dye Surface — **Yanlin Qin, Xuliang Lin, Yufei Ma, Yanxiang Fang, Tiejun Wang**

**Paper 6af:** Elastohydrodynamics and Soft Matter Mechanics to Understand Biological Adhesion, Human Touch, and Optics-Free Cytometry — **Charles Dhong**

**Paper 6jo:** Using Microbotic Tools for Probing Cellular Pattern Generation and Morphogenesis — **Sambeeta Das**

**Paper 6jm:** 3D Bio-Printed Models of Vascularized Tissues — **Vivian K. Lee**

**Paper 6jv:** From Macromolecular Science to the Skin Barrier: Engineering Novel Platforms for Transdermal Drug Delivery — **Mohammad Mofidfar**

**Paper 6kc:** Soft, Stretchable Wearable Platforms for Sensing and Energy Harvesting Applications — **Amay J. Bandodkar, Joseph Wang, John A. Rogers**

**Paper 6ag:** Genetically Engineered Probiotics to Target and Eliminate Colorectal Cancer — **Amin Zargar**



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.



## ■ BIOMEDICAL ENGINEERING

**Paper 6ai:** Engineered Hydrogel Biomaterials for Mimicking Tumor Microenvironments and Controlling Cancer Cell Fate — **Shantanu Pradhan, John Slater**

**Paper 6aj:** Interstitial Fluid Flow and Transport in Neural Trauma and Disease — **R. Chase Cornelison**

**Paper 6ak:** Quantitative Label-Free Dynamic Phenotyping of Highly Metastatic Cancer Cells for Emerging Liquid Biopsy Applications — **Jose C. Contreras-Naranjo**

**Paper 6al:** Biofilm Engineering for Human Health and Environmental Sustainability — **Abdelrhman Mohamed, Haluk Beyenal**

**Paper 6am:** Multi-Scale Biomolecular Modeling and Design for Engineering and Medicine — **Chris A. Kieslich**

**Paper 6an:** Design and Development of Point-of-Care Microsystems for Diagnosis of Neurodegenerative Diseases — **Jae Hwan Jung**

**Paper 6ao:** In Vitro Microphysiological Systems for Disease Modeling, Drug Development, and Regenerative Medicine — **Ying Wang**

**Paper 6ap:** Electrochemical Biotechnology — **Ariel Furst**

**Paper 6aq:** From Cells to Tissues : Understanding Development, Evolution and Disease Using Single-Cell RNA-Sequencing — **Karthik Shekhar**

**Paper 6ar:** Daniel Cook - Understanding and Treating Progressive Diseases at the Levels of Single Cells and Single Patients Through Systems Biology — **Daniel Cook**

**Paper 6as:** Decellularization Approaches to Engineering Test Beds of Health and Disease — **Young Hye Song**

**Paper 6at:** Application of Room Temperature Ionic Liquids in Membrane Based Technology: An Unconventional Green Separation — **Arijit Sengupta**

**Paper 6ajk:** Assessing Role of Signaling Network Properties at the Immune System and Cancer Nexus — **Shibin Mathew**

**Paper 6iwi:** Leveraging Big Data and Engineering Fundamentals Towards Biological Discovery — **Purushottam Dixit**

## ■ CATALYSIS

**Paper 6au:** Computational Insights into Zeolite-Catalyzed Biomass Conversion to Olefins — **Sha Li**

**Paper 6av:** Engineering Catalytic and Reactive Interfaces for the Sustainable Production of Fuels and Chemicals — **Melis S. Duyar**

**Paper 6aw:** Catalytic CO<sub>2</sub> Conversion to Clean Fuels and Chemicals: Integration of Traditional Metallic Catalysts and Metal-Organic Frameworks — **Xiao Jiang**

**Paper 6ax:** Synergizing Model Surfaces and Real Catalysts for Efficient Electrochemical Energy Conversion — **Andrew Akbashev**

**Paper 6ay:** Mixed-Metal-Oxide Redox-Catalyst for Shale-Oil and Gas Conversion — **Luke Neal**

**Paper 6az:** The Synergistic Effect of Copper and Niobium Species on a Novel Cu/Nb-Ti Mixed Oxide Catalyst for the Selective Catalytic Reduction of NO<sub>x</sub> with NH<sub>3</sub> — **Xiaoxiang Wang, Liang Chen, Wei Li, Yao Shi, Su-Jing Li**

**Paper 6ba:** Fabrication of Fe-ZSM-5@CeO<sub>2</sub> Catalysts with a Core-Shell Structure and the Enhanced Performances for the Selective Catalytic Reduction of NO with NH<sub>3</sub> — **Liang Chen, Xiaoxiang Wang, Wei Li, Su-Jing Li**

**Paper 6bb:** Combining Theory and Experiment at the Electrode/Electrolyte Interface to Improve Electrochemical Energy Conversion and Storage — **Ian T. McCrum**

**Paper 6bc:** Optimizing Electrocatalysts for Energy Storage and CO<sub>2</sub> Conversion — **Brian M. Tackett**

**Paper 6bd:** Nature of Active O<sub>2</sub>-Derived Species in Selective Oxidation Catalysis — **Stephanie Kwon**

**Paper 6be:** Fundamental Understanding of Non-Traditional Feedstock Conversion Processes — **Hilal Ezgi Toraman**

**Paper 6bf:** Decoding the Complexity of Chemical Reactions on Single Atom Catalysts and Beyond — **Konstantinos Alexopoulos**

**Paper 6bg:** Catalysis Informatics: Accelerating Search and Discovery of New Catalysts — **Jacob R. Boes**

**Paper 6bh:** Molecular Modeling and Machine Learning for Catalysis and Separations — **Tyler R. Josephson**

**Paper 6bi:** Novel Catalytic Materials for Efficient Chemistry - Elucidation of Fundamental Structure-Activity Relationships — **Madelyn R Ball**

**Paper 6bj:** Controlled Catalytic Capability through Tailored Nanoporous Materials: For Selective and Sustainable Chemical Processes — **Hong Je Cho**

**Paper 6bk:** Advanced Materials for Efficient Energy Conversion Based on Spectroscopic and Mechanistic Study — **Xuan Yang**

**Paper 6bl:** Combining Heterogeneous Catalysis and Surface Science. Green Processes and Energy Applications — **David Martin Alonso**

**Paper 6bm:** Bridging Concepts between Electrochemically and Thermally Activated Catalytic Reactions — **Joaquin Resasco**

**Paper 6bn:** Designing Catalysts for Conversion of Alternative Carbon Feedstocks to Fuels and Chemicals — **Siddharth H. Krishna**

**Paper 6bo:** Catalysts for Sustainable Processes: Understanding and Controlling Active Site Environments — **David Chester Upham**

**Paper 6bp:** Bimetallic Catalysis for Various Shale Gas and Biomass Conversions — **Yang Xiao, Arvind Varma**

**Paper 6bq:** Enzymatic Reaction Induced Protocell Motility — **Woo-Sik Jang, Hyun Ji Kim, Chen Gao, Daeyeon Lee, Daniel A. Hammer**

**Paper 6br:** Environmental Applications of Al/Zr Pillared Clay As Efficient Heterogeneous Catalyst for Catalytic Wet Oxidation of Phenol — **Siwela Jeffrey Baloyi**

**Paper 6bs:** Electrochemical Strategies for Sustainable Energy Technologies — **Joshua M. McEnaney**

**Paper 6bt:** High-Throughput Catalysts Screening of Layered Double Hydroxides for Oxygen Evolution and Reduction Reactions — **Zhenghang Zhao, Ambarish R. Kulkarni, Michal Bajdich, Jens Nørskov**

**Paper 6bu:** Heterogeneous Catalysts Development for Benzene Saturation in Diesel — **Shyamal Roy**

**Paper 6bv:** The OH--Controlled Synthesis of Pt-Ni Nanocatalysts with Different Atomic Distributions for Alkaline Hydrogen Evolution Reaction — **Cong Zhang, Biaohua Chen, Xin Liang**

**Paper 6bw:** Catalytically Active and Hazardous Gas Adsorbent Polymer Fibers Functionalized By Atomic Layer Deposition and Metal-Organic Framework Thin Films — **Dennis T. Lee, Gregory N. Parsons**

**Paper 6bx:** Nife Layered Double Hydroxide/Hollow Prussian Blue Via Alkaline Etching As an Efficient Electrocatalyst for Oxygen Evolution Reaction — **Xinran Zhao, Biaohua Chen, Fengxiang Yin, Xiaobo He**

**Paper 6by:** Synthesis of 5-Hydroxymethylfurfural from Disaccharides Using Niobium-Modified Montmorillonite — **Guo Qiu, Biaohua Chen, Chongpin Huang**

**Paper 6bz:** Synthesis of Organometallic Single-Site Heterogeneous Catalysts for Sustainable Chemistry — **Jacob Heltzel, Adelina Voutchkova-Kostal**

**Paper 6ca:** Catalysis for Sustainability: Probing the Fundamentals of Chemical Conversion Using Synthetic, Kinetic, and Electrocatalytic Approaches — **Mark Sullivan**

**Paper 6cc:** Photocatalytic and Electrocatalytic Reduction Process of CO<sub>2</sub> with H<sub>2</sub>O to CH<sub>3</sub>OH over Bismuth-Promoted Perovskite-Based BaTiO<sub>3</sub> Catalyst — **Venkata Dasireddy, Blaž Likozar, Shizhang Qiao**

**Paper 6cd:** Rational Design of Pt-Ni Catalysts for the Oxygen Reduction Reaction By Building Atomic-Scale Structure-Property Relationships — **Liang Cao**

**Paper 6ce:** Enabling Concepts in Catalysis Science — **James W. Harris**

**Paper 6cf:** Photocatalytic and Electrocatalytic Reduction Process of CO<sub>2</sub> with H<sub>2</sub>O to CH<sub>3</sub>OH over Bismuth-Promoted Perovskite-Based BaTiO<sub>3</sub> Catalyst — **Venkata Dasireddy, Blaž Likozar, Shizhang Qiao**

**Paper 6cg:** Unraveling the Mechanism of the Oxidation of Glycerol to Dicarboxylic Acids over a Sonochemically Synthesized Copper-Oxide Catalyst — **Prince N. Amaniampong**

**Paper 6ch:** Single-Molecule Organometallic Catalysis, and Fluorescent Materials Preparation and Application — **Xiangcheng Sun**

**Paper 6ji:** Discovery and Development of Biocatalysts for Fine Chemicals Synthesis — **Peng Wang**

**Paper 6jt:** Catalyst Studies on the Conversion of Biobased Intermediates to Biobased Products — **Iman Nezam**



**Paper 6ka:** Process Intensification Driven Catalysts Development for CO<sub>2</sub> Utilization and Drop-in Fuels Production from Renewable Feedstock — [Chinmoy Baroi](#)

## ■ COMPUTATION & MODELING

**Paper 6ci:** New Frontiers in Process Systems Engineering for Large Multiscale Chemical and Energy Networks — [Andrew Allman](#)

**Paper 6cj:** Toward Autonomous Molecular Discovery: Machine Learning and Automation for the Rational Design and Optimization of Novel Compounds — [Connor W. Coley](#)

**Paper 6ck:** Understanding and Exploiting the Tunability of Long-Range Electrostatic Interactions in Soft Materials — [Meng Shen](#)

**Paper 6cl:** Molecular Modeling of Anti-Microbial Peptides at a Water-Lipid Bilayer Interface — [Faramarz Joodaki](#)

**Paper 6cm:** Computational Design of Functional Materials and Their Interfaces — [Tibor Szilvási](#)

**Paper 6cn:** Multi-Scale Modeling of Biophysical Systems and Soft Matter — [Harshwardhan H. Katkar](#)

**Paper 6co:** Toward Emergent, Adaptive, and Hierarchical Bio-Inspired Materials — [Alexander J. Pak](#)

**Paper 6cp:** Multiscale Simulations of Nonequilibrium Mechanisms in Aqueous Solutions — [Aviel Chaimovich](#)

**Paper 6cq:** Computational Design and Characterization of Nanoscale Materials for Applications in Energy, Separations, and Catalysis — [N. Scott Bobbitt](#)

**Paper 6cr:** Data-Driven Modeling in Chemical Engineering and Molecular Science — [Joseph S. Gomes](#)

**Paper 6cs:** Process Systems Engineering and Artificial Intelligence for Advanced Manufacturing: Including Applications to Biopharmaceuticals — [Yu Luo](#)

**Paper 6ct:** Optimization in Three Process System Engineering Problems: Inventory Routing, Product Scheduling and Design of Experiments — [Yachao Dong](#)

**Paper 6jp:** Designing Chemical Reactivity at the Nanoscale using Molecular Simulation — [Ryan Gotchy Mullen](#)

**Paper 6js:** Theories and Simulations for Liquid-Liquid Phase Separation in Biology — [Yi-Hsuan Lin](#)

## ■ ELECTROCHEMISTRY

**Paper 6cu:** Materials Discovery for Energy and Environmental Applications Using First-Principles Multiscale Simulations — [Mudit Dixit](#)

**Paper 6cv:** Engineering Electrocatalysts for Sustainable Energy Technologies: From Theory to Rational Design through in-Situ Characterization — [Mohammad Norouzi Banis](#)

**Paper 6cx:** Novel Electrokinetic Solutions for Energy and Environmental Problems — [Mohammad Mirzadeh, Martin Z. Bazant](#)

**Paper 6cy:** Electrocatalysis for Sustainable Energy Storage and Conversion — [Laurie A King](#)

**Paper 6cz:** Understanding and Controlling Multielectron Transfer Electrochemistry Toward Sustainable Energy Technologies — [Adam Nielander](#)

**Paper 6da:** Electrochemical Plasma Reactions and Supersonic Printing: A Route Towards Multi-Component Materials Discovery and Scalable Device Manufacturing — [Souvik Ghosh](#)

**Paper 6dc:** Development of Devices and Selective Catalysts for the Solar-Driven Electrochemical Reduction of CO<sub>2</sub> to Fuels — [Marcel Schreier, Michael Grätzel, Yogesh Surendranath](#)

**Paper 6dd:** Electrochemical Ion Insertion: Mechanisms and Applications in Energy Storage and Computing — [Yiyang Li](#)

**Paper 6df:** A Fundamental Understanding of CO<sub>2</sub> Electrolysis Using Synchronous X-Ray Studies — [Xueli Zheng, Yi Cui](#)

## ■ ENERGY, SUSTAINABILITY, & THE ENVIRONMENT

**Paper 6dg:** Research on the Structure Design and the Flow Field Characteristics of Supersonic Separator — [Huirong Liang, Shuai Zhang, Yong Kang, Lu Yang](#)

**Paper 6dh:** Nanostructured 2D Carbides and Nitrides for Electrochemical Energy Storage and Conversion — [Abdoulaye Djire](#)

**Paper 6di:** Flame-Made Nanoparticles: Morphology, Optical Properties and Climate Impact — [Georgios A. Kelesidis](#)

**Paper 6dj:** Multi-Scale Modeling of the Structure and Dynamics of Bio-Inspired Light-Harvesting Technologies — [William P. Bricker](#)

**Paper 6dk:** Techno-Economic Analysis and Optimization for Energy Storage Systems — [Naresh Susarla](#)

**Paper 6dl:** Atomistic Modeling of Energy Storage Materials — [Jeffrey S. Lowe, Donald J. Siegel](#)

**Paper 6dm:** Optimal Carbon Capture and Storage Network Based on First-of-a-Kind (FOAK) and Nth-of-a-Kind (NOAK) Economic Analysis — [In-Beum Lee](#)

**Paper 6dn:** Fit Batteries to the Grid or Grid to the Batteries? — [Seong Beom Lee, Venkat R. Subramanian](#)

**Paper 6do:** Advanced Materials and Nanotechnologies for Efficient, Solution Processable Energy Devices — [Tze-Bin Song](#)

**Paper 6dp:** Design and Development of Materials and Electrolytes for Energy: From Fundamental Mechanisms to Applications — [Maria Lukatskaya](#)

**Paper 6dq:** Exploring the Solid-Electrolyte Interface and Interphase By Surface-Plasmon Resonance Spectroscopy — [Guang Yang, Jagjit Nanda](#)

**Paper 6dr:** Hydrothermal Technologies for Valorizing Biomass and Producing Valued-Added Chemicals — [James D. Sheehan](#)

**Paper 6ds:** All-Solid-State Batteries for Next Generation Electrochemical Energy Storage — [Fudong Han](#)

**Paper 6dt:** Organic Molecular Electrocatalysts for Energy-Water Applications — [Xi Yin](#)

**Paper 6du:** Experimental Investigation on Different Baffles of Shell-and-Tube Heat Exchanger — [Tao Cheng, Jian Chen, Min Zeng](#)

**Paper 6dv:** A Reduced Combustion Kinetic Model for the Methanol/Methane Dual-Fuel Engine — [Qingang Zhang](#)

**Paper 6dw:** Experiment on the Performance of Natural Gas/Methanol Dual-Fuel Engine — [Qingang Zhang, Zhanming Chen, Ke Zeng](#)

**Paper 6dx:** Three-Dimensional Numerical Simulation of Natural Gas/Methanol Dual-Fuel Engine — [Qingang Zhang, Zhanming Chen](#)

**Paper 6dy:** Electrolyte Design and Fundamental Studies of Battery Systems for Better Energy Storage Media — [Chibueze Amanchukwu](#)

**Paper 6dz:** Systems Approaches to Design Sustainable Food-Water-Energy-Waste Nexus Processes and Systems — [Daniel Garcia](#)

**Paper 6ea:** Sustainable Fuel and Chemical Synthesis Via Catalytic Valorization of Abundant and Renewable Resources — [Nathaniel Eagan](#)

**Paper 6ec:** Kinetics and Reliability of Thermo-Electro-Chemical Processes for Energy Conversion and Chemical Production — [Xiao-Yu Wu](#)

**Paper 6ed:** Fueling Our Future with Membrane Technology: Clean Energy Conversion and Process Intensification — [Simona Liguori](#)

**Paper 6ee:** Electromagnetic and Chemical Treatment for Efficient Multiphase Petroleum Transportation — [Yingda Lu](#)

**Paper 6ef:** Applications of Functional Fiber-Based Materials in Energy and Engineering Fields — [Jiadeng Zhu](#)

**Paper 6eg:** Nanoscale Solid State Electrolyte Synthesized through Atomic Layer Deposition for Interfacial Engineering and All-Solid-State Batteries — [Chuan-Fu Lin, Gary W. Rubloff](#)

**Paper 6eh:** Energy Storage in Clathrate Hydrates – Recent Advancements in Solidified Natural Gas (SNG) Technology — [Hari Prakash Veluswamy](#)

**Paper 6ei:** Clathrate Hydrates for Sustainable Development — [Ponnivalavan Babu](#)

**Paper 6ej:** Modeling the UV/H<sub>2</sub>O<sub>2</sub> Oxidation of Trace Organic Compounds in a Continuous-Flow Reactor with Reflective Walls — [Tianqi Zhang, Itzel Marquez, Robert Arnold, George Diefenthal, Eduardo Sáez](#)

**Paper 6ek:** Thermal Degradation of Morpholine for CO<sub>2</sub> Capture — [Shaukat Ali](#)

**Paper 6el:** Metal-Free Organic Molecular Electrocatalysts for Energy Applications — [Xi Yin](#)

**Paper 6em:** Construction of Ultrasonic / Magnetic Combined Reactor for Rapid Clarification of Turbid Metamorphic Diesel Oil — [Mubarak Abolore Azeez](#)

**Paper 6en:** Fundamental Discovery and Materials Design for Energy Storage — [Yuzhang Li, Yi Cui](#)

**Paper 6eo:** Reinforced Anion Exchange Membrane (AEM) Separators Based on Triblock Copolymers for Electrode-Decoupled Redox Flow Batteries (RFBs) — [Shrihari Sankarasubramanian](#)

**Paper 6jy:** Rational Design of Novel Catalysts for Energy Applications — [Zhiqiang Ma](#)

**Paper 6jz:** Sustainable Production of Renewable Specialty Chemicals and Fuels from the Catalytic Conversion of Lignocellulosic Biomass — [Oscar Oyola-Rivera](#)

## ■ FLUID MECHANICS

**Paper 6ep:** Control of Slip at the Fluid-Surface Interface Using Molecular Additives — [Fardin Khabaz](#)

**Paper 6eq:** Engineering Non-Equilibrium Materials with Controllable Spatiotemporal Patterns: Oscillator Networks and Active Suspensions — [Michael M. Norton](#), [Zvonimir Dogic](#), [Aparna Baskaran](#), [Michael F. Hagan](#), [Seth Fraden](#)

**Paper 6er:** Dynamic Microstructure and Interactions in Complex Fluids Under Flow and Confinement — [John Riley](#)

**Paper 6es:** Complex Interfacial Dynamics, Deformation-Based Microrheology, and Beyond — [Harishankar Manikantan](#)

**Paper 6et:** Fluid Dynamics at Different Length Scales in Confinements — [Shima Parsa](#), [David A. Weitz](#)

**Paper 6eu:** Coalescence, Spontaneous Emulsification and Submerged Coffee Rings in the Presence of Asphaltene Adsorption — [Simone Bochner de Araujo](#), [Gerald G. Fuller](#)

**Paper 6ev:** Research on the Vertical Falling Film Behavior in the Scrubbing-Cooling Tube — [Yifei Wang](#), [Xin Peng](#), [Liucheng Yan](#), [Guangsuo Yu](#), [Fuchen Wang](#)

**Paper 6ew:** Fluid Mechanics of Two-Phase Flows: Concentrated Suspension of Non-Spherical and Deformable Particles — [Sarah E. Mena](#)

**Paper 6ex:** Active Soft Matters and Soft Interfaces — [Mehdi Molaei](#)

**Paper 6ey:** Experimental and Numerical Studies on the Micromixing Process in Novel Reactors with Multiphase System — [Yi Ouyang](#), [Hai-Kui Zou](#), [Guang-Wen Chu](#), [Yang Xiang](#), [Ramesh Agarwal](#), [Jian-Feng Chen](#)

**Paper 6jl:** Multiscale Computation of Microscale Fluid Dynamics in Porous Materials — [Yashar Mehmani](#), [Hamdi Tchelepi](#)

## ■ INTERFACIAL & TRANSPORT PHENOMENA

**Paper 6ez:** From Liquid Crystalline Solutions to Functional Materials — [Vida Jamali](#)

**Paper 6fa:** Modeling across Disparate Spatiotemporal Scales – Enabling Answers to Grand Engineering Challenges — [Dwaipayan Dasgupta](#)

**Paper 6fb:** Engineering Nanoscale Materials and Interfaces for Sustainable Energy and Chemical Processes — [Matthew A. Gebbie](#)

**Paper 6fc:** Designing Functional Soft Materials Using Anisotropic Fluids — [Karthik Nayani](#)

**Paper 6fd:** Transport Phenomena at Microscopic Scales and Their Effects on Macroscopic Scale Processes — [Thao Nguyen](#)

**Paper 6ff:** Laboratory of Interfaces, Flow and Electrokinetics (LIFE) — [Ankur Gupta](#)

**Paper 6fg:** Achieving Next-Level Transport with Soft Matter and Interfaces — [H. Jeremy Cho](#)

**Paper 6fh:** Numerical Studies on Granular Flows at Macroscopic and Microscopic Levels Using DEM — [Jiecheng Yang](#), [Yu Guo](#), [Jennifer S. Curtis](#)

**Paper 6fi:** Application of Gas Hydrate Slurry Relative Viscosity Models for an Advanced Hydrate Management Strategy — [Ahmad Abdul Majid](#), [David T. Wu](#), [Carolyn A. Koh](#)

## ■ MATERIALS

**Paper 6fk:** From Training in Polymer Physics to Developing Nonwovens for Advanced Applications — [Behzad Nazari](#)

**Paper 6fl:** Continuous Technology Platforms Enabled By Molecular Design of Disperse Multiphase Soft Matter — [Abu Zayed Md Badruddoza](#)

**Paper 6fm:** Self-Assembly, Elasticity, and Rheology of Soft Materials — [Rodrigo Guerra](#)

**Paper 6fn:** New Frontiers in Materials Chemistry for Sustainable Energy Technologies — [Andrew B. Wong](#)

**Paper 6fo:** Design and Fabricate Functional Materials for Biological and Energy Applications — [Weixia Zhang](#)

**Paper 6fp:** Using in-Situ X-Ray Analysis Techniques to Understand Materials Synthesis — [Bor-Rong Chen](#)

**Paper 6fq:** Radical-Bridged Dinuclear, Trinuclear and Metallocyclic Lanthanide Molecular Magnets — [Brian Dolinar](#)

**Paper 6fr:** Soft Materials and Bio-Integrated Devices: From Complex Colloidal Systems to Skin/Brain-Interfaced Biosensors — [Yi Zhang](#)

**Paper 6fs:** Porous, Conductive Crystals: Expanding the 2D Materials Library with Metal-Organic Frameworks (MOFs) — [Robert Day](#)

**Paper 6fu:** Sheikh Laboratory for Sustainable Soft Matter and Active Interfaces — [Amir Sheikh](#)

**Paper 6fv:** Programmable 3D Transformation of Smart Soft Materials — [Ji-Hwan Kang](#)

**Paper 6fw:** Harnessing Flow-Microstructure Interactions Towards Improved Soft Materials Manufacturing and Processing — [Antonio Perazzo](#)

**Paper 6fy:** Engineering Transport in Microporous Materials for Next-Generation Energy Technologies — [Jonathan E. Bachman](#)

**Paper 6fz:** Engineering Complex Polymer Materials with Tailored Chemistry, Morphology, and Functionality — [Caroline Szczepanski](#)

**Paper 6ga:** Multifunctional Soft-Nano Interfaces for Energy, Environment, and Healthcare — [Kunal Mondal](#), [Michael D. Dickey](#), [Jan Genzer](#), [Ashutosh Sharma](#)

**Paper 6gb:** Building Hierarchical Materials for Energy and Catalysis — [Xin Zhang](#)

**Paper 6gc:** Ionic and Electronic Transport Properties in Bulk and Nano Metal Oxides — [Ankit Agrawal](#)

**Paper 6gd:** Machine Learning and Data-Enabled Design and Discovery of Nano and Soft Materials — [Tarak Patra](#)

**Paper 6ge:** Sustainable Materials for Separations and Catalysis — [William P. Mounfield III](#)

**Paper 6jr:** Task-Specific Functional Porous Materials: From Academic Laboratory to the Commercial Marketplace — [Sameh Elsaïdi](#)

**Paper 6jw:** Engineering Soft Materials with Different Length Scales for Diversity Applications — [Liyuan Zhang](#), [David A. Weitz](#)

**Paper 6kb:** Advanced Deposition and Characterization of Thin Films for Electronics and Sustainable Energy — [Sean L. Berglund](#)

**Paper 6kd:** Colloidal Templating of Model Mesostructured Surfaces for Electrochemistry, Optics, and Sensing — [Katherine Phillips](#)

## ■ NANOMATERIALS & NANOTECHNOLOGY

**Paper 6gf:** Nanoengineering Materials with Atomic Specificity for Catalysis and Energy Applications — [Tej S. Choksi](#)

**Paper 6gg:** Strategic Advancement of Targeted Nanomedicines: Intelligent Bio-Nanoengineering Using Molecular Imaging in 3D and *In Vivo* tumor Models — [Girgis Obaïd](#)

**Paper 6gh:** Utilizing Nano- and Micro-Particles for Safe and Efficient Gene and Drug Delivery — [Brittany E. Givens](#)

**Paper 6gi:** Engineering Optical Nanomaterials to Probe Brain Chemistry — [Jackson Travis Del Bonis-O'Donnell](#)

**Paper 6gj:** Reprogramming Tumor-Clearing Macrophages with Nanotherapeutics — [Fan Zhang](#)

**Paper 6gk:** Complex Nano-Architectures from Self-Assembly and Surface-Confined Chemistry for Energy Storage and Beyond — [Jörg G. Werner](#)

**Paper 6gl:** Continuous Manufacturing of Ultrathin Electronic/Optoelectronic Devices with Colloidal Nanocrystals — [Hyeong Jin Yun](#)

**Paper 6gm:** Toward Next Generation of Colloidal 2D Nanomaterials: Liquid-Phase Characterization, Modification, and Controlled Assembly — [Dorsa Parviz](#)

**Paper 6gn:** A Comprehensive Study of Photocatalytic Degradation of Methylene Blue By ZnO Nanoparticles and Its Nano-Composites with Ag an C<sub>3</sub>N<sub>4</sub> Under UV Light — [Sadia Ata](#), [Samina Ghafoor](#), [Irfah Mirza](#), [Quratul Ayn](#)

**Paper 6go:** Novel Nanomaterials for Chemical and Life Sciences — [Rajendar R. Mallepally](#)

**Paper 6gp:** Design of Functional Nanomaterials for Energy Applications Using Flow Reactors — [Ioannis Lignos](#)

**Paper 6gq:** Structural and Electronic Transformations in Dynamic Semiconductor Nanomaterials — [Clayton Dahlman](#)

**Paper 6gr:** Engineering Multifunctional Nanomaterials for Energy and the Environment — [Michael Bozlar](#)

**Paper 6gs:** Taking the Lab to the Field: Performing Real-Time Environmental and Diagnostic Monitoring — [Lynn E. Secondo](#)

**Paper 6gt:** Iron Oxide Nanoparticles Inhibit Metastasis and Tumor Growth in Lung — [Saeid Zanganeh, Morteza Mahmoudi](#)

**Paper 6gu:** Cell Shape: An Overlooked Factor at the Nanobio Interfaces — [Morteza Mahmoudi, Saeid Zanganeh](#)

**Paper 6gv:** Nano-Bionics: Polymer and Metal-Organic Thin Films and Particles for Engineering Life — [Joseph J. Richardson](#)

**Paper 6gw:** Materials Chemistry As Engineering Solutions: Metamaterials, Energy and Water — [Yoonseob Kim, Timothy Swager, Nicholas A. Kotov](#)

**Paper 6gx:** Electricity from Asymmetric Chemical Doping — [Albert Tianxiang Liu, Michael Strano](#)

**Paper 6gy:** Chiral Nanostructures: Design Strategies and Their Properties — [Jihyeon Yeom, Nicholas Kotov, Robert Langer](#)

**Paper 6gz:** Assembly Engineering for Bio-Inspired Nanomaterials — [Trung Nguyen](#)

**Paper 6ha:** Nano Engineering with X-Ray through Infrared Spectroscopy (NEXIS) — [Zachary Fishman](#)

**Paper 6hb:** Engineering Nanopores and Nanostructures of Atomically Thin Sheets and Carbon Nanotubes — [Daichi Kozawa](#)

**Paper 6hd:** Tuning Complex Fluids from the Nanoscale — [Sara M. Hashmi](#)

**Paper 6he:** Nanocomposites Synthesis, Characterization and Its Application in Energy, Environment and Healthcare — [Mausumi Mukhopadhyay](#)

**Paper 6ju:** Functional 2D Material Nanoarchitectures for Sustainable Energy Generation — [Sanjay Behura](#)

## ■ PARTICLE TECHNOLOGY

**Paper 6hf:** Experimental and Numerical Investigations of Particle Flows — [Casey Q. LaMarche](#)

**Paper 6hg:** Dynamic Structures in Multiphase Systems: A Pathway Towards Responsive Processes — [Victor Francia](#)

**Paper 6hh:** Effects of Complex Particle Interactions on Fluid-Particle Flows — [Jari Kolehmainen](#)

**Paper 6hi:** Two-Component Polymeric Systems That Provide High Performance, Easy Operation, Environmental Friendliness, and Health Benefits — [Guozhen Yang](#)

## ■ POLYMERS

**Paper 6hk:** Reconfigurable Polymers for Advanced Materials Applications — [Deborah K. Schneiderman](#)

**Paper 6hl:** Modeling Transport and Rheology in Polymers and Particle-Polymer Mixtures to Enable the Rational Design of Novel Soft Materials — [Christian Aponte-Rivera](#)

**Paper 6hm:** Understanding the Remarkable Physical Chemistry of Novel Polymer Materials: How Does Intricate Chemical Functionality Enhance Material Properties? — [Raim Ricarte](#)

**Paper 6hn:** Understanding and Controlling Self-Assembly in Polymer and Colloidal Systems through Simulation, Theory, and Experiment — [Thomas Gartner III](#)

**Paper 6ho:** Designing New Functional Soft Materials with Molecular Simulations — [Antonia Statt](#)

**Paper 6hp:** Nanostructural Engineering Towards on-Demand Manipulation of Polymers and Their Derivatives Functionality — [Zhe Qiang](#)

**Paper 6hq:** From Chemical Bond Forces and Breakage to Macroscopic Fracture of Soft Materials — [Gabriel E. Sanoja](#)

**Paper 6hr:** Gradient Double Network Gels for Medical Implants — [Pandiyarajan Chinnayan Kannan](#)

**Paper 6hs:** Structure and Design of Soft Materials for Stretchable Electronics — [Seunghyun Sung](#)

**Paper 6ht:** Transport and Structure in Polymer Membranes for Energy-Efficient Separations — [Hee Jeung Oh](#)

**Paper 6hu:** Synthetic Polymeric Materials for Energy Storage and Gas Separation — [Pengfei Cao, Alexei Sokolov, Tomonori Saito](#)

**Paper 6hv:** Functional Designer Polymers for Integrating Advanced Synthetic and Biological Materials — [Jeffrey M. Ting](#)

**Paper 6hx:** Multiscale Structure and Dynamics of Polymers and Biological Soft Matter — [Danielle J. Mai](#)

**Paper 6hy:** Designing Polymers As Molecular Recognition Agents for Diagnostic Biosensing and Imaging — [Heidi R. Culver](#)

## ■ PROCESS DESIGN, DEVELOPMENT, & CONTROL

**Paper 6hz:** Process Design and Optimization Leveraging Multiscale Modeling and Machine Learning — [Hanyu Gao](#)

**Paper 6ia:** Building a New Computational Toolbox for Bioengineering and Advanced Manufacturing — [Robert J. Lovelett](#)

**Paper 6ib:** Process System Engineering (PSE): *Continuous Pharmaceutical and Bio-Pharmaceutical Manufacturing* — [Ravendra Singh](#)

**Paper 6ic:** Novel Strategies for Real-Time Stochastic Optimization, Quantification of Model Uncertainty and Estimation of the Physical Properties of Biologics — [Francesco Rossi, Flavio Manenti, Guido Buzzi-Ferraris, Gintaras Reklaitis](#)

**Paper 6id:** Optimization-Based Control of Complex Process Networks in Smart Manufacturing: The Appearance of Cyber-Physical Systems, Cloud Computing, and Big Data Analytics — [Davood Babaei Pourkargar](#)

**Paper 6ie:** Development and Assessment of New Sustainable Processes for the Production of Bio-Products — [Sampath Gunukula](#)

**Paper 6if:** An Open Source Process Simulation Environment on Python for Automated Preliminary Techno-Economic Analysis — [Yoel Cortes, Deepak Kummur, Vijay Singh, Jeremy Guest](#)

**Paper 6ig:** Optimal Design of Petroleum Refinery Configuration Using a Model Based Mixed-Integer Programming Approach with Practical Approximation — [Tareq Albahri, Cheng Seong Khor, Mohamed Eisholkami, Ali Elkamel](#)

**Paper 6ij:** Active Process Control in Pharmaceutical Continuous Manufacturing — the Quality By Control (QbC) Paradigm — [Qinglin Su](#)

## ■ SEPARATIONS

**Paper 6ij:** High Performance Polymers for Water Purification and Energy Storage/Generation Applications: Rational Design Guided By Fundamental Structure/Property Relations — [Jovan Kamcev](#)

**Paper 6ik:** Molecule Separation and Conversion Using Novel Porous Material — [Jian Liu](#)

**Paper 6il:** Engineering Anisotropy a New Design Strategy for Membrane Gas Separations — [Juan Manuel Restrepo-Florez, Martin Maldovan](#)

**Paper 6im:** Energy-Efficient Membrane-Based Separations — [Canghai Ma](#)

**Paper 6in:** Membrane Technology and Bioengineering for Sustainable Products and Processes — [Saurav Datta](#)

**Paper 6io:** Morphology Engineering of Carbon Molecular Sieve Membranes for Advanced Separations — [Oishi Sanyal](#)

**Paper 6ip:** Advanced Porous Materials for Scalable Molecular Separation: Integration of Material, and Process, and Engineering — [Kiwon Eum](#)

## ■ SYNTHETIC BIOLOGY

**Paper 6iq:** Synthetic Post-Translational Circuits for Cell-Mediated Therapy of Diseases Involving Immune Dysfunction — [Nichole Daringer](#)

**Paper 6ir:** Engineering a Purple Non-Sulfur Bacterium to Expand Symbiotic Nitrogen Fixation — [Cheryl Immethun](#)

**Paper 6is:** Proteins Nanoparticles with Control of Shape, Size, and Valency for Therapeutics — [Kevin Metcalf](#)

**Paper 6it:** Biosensor Mediated Evolution of Biosynthetic Pathways for Biomanufacturing — [Niju Narayanan](#)

**Paper 6iu:** Cell-Free Bioprocess Engineering for a Renewable Carbon Future — [Joseph Rollin](#)

**Paper 6iv:** Stochasticity, Complexity, and Multiscale Dynamics in Cancer Progression and Drug Response — [Leonard A. Harris](#)

**Paper 6ix:** Biomolecular Engineering and Magnetic Resonance for Structural Biology and Synthetic Biology — [George J. Lu](#)

**Paper 6iy:** Expanding the Biosynthetic Potential of Living Systems — [Jorge Marchand](#)

**Paper 6iz:** Single-Cell Analysis for Advancing Synthetic Biology — [Leqian Liu](#)

**Paper 6jx:** Application of Advanced Synthetic Biology Tools to Genetic Engineering and Bioprocessing — [Jicong Cao](#)



## ■ THERMODYNAMICS

**Paper 6ja:** A Group Contribution Method for Heat Capacity Estimation of Hydrocarbons — *Yizhen Song, Xiaoming Zhao*

**Paper 6jb:** Theoretical Calculation of Ethane Thermal Cracking Temperature — *Yizhen Song, Xiaoming Zhao*

**Paper 6jc:** Protein-Protein Hydrodynamics & Thermodynamics in Concentrated Solutions and Therapeutic Protein Stability in Manufacturing-Relevant Flow Fields — *Jai A. Pathak*

**Paper 6je:** Using X-Ray Science to Study Structure and Ultrafast Dynamics in Liquids — *Harshad Pathak*

**Paper 6jf:** Molecular Simulations of Biological Self-Assembly — *Gul H. Zerze*

**Paper 6jg:** Multi-Dimensional Single Cell Analysis with a Chemistry, Materials, and Nanotechnology Toolset — *Alex Xu*

**Paper 6jh:** Multiscale Simulation Studies of Polymers, Ionic Liquids, Biopolymers and —

**Paper 6jq:** Life-Cycle and Techno-Economic Assessment of Microalgal Biorefinery for Biological CO<sub>2</sub> Sequestration — *Geetanjali Yadav*

### (7) Entrepreneurship & Investing in Early-Stage Chemical Companies

**Sunday, Oct 28, 2:30 PM**

Westin Convention Center, Cambria

**Sponsored by:** Miscellaneous

**2:30 Paper 7a:** Angel Investing in the Hard Sciences - Chemical Angel Network (CaN) — *Mark Vreeke*

**2:45 Paper 7b:** Incubator Operations — *Mark Vreeke*

**3:05 Paper 7c:** Why I'm an Angel Panel Introduction — *Mark Vreeke*

**3:10** Panelist 1 - William Byers, CaN Member & Past President, AIChE

**3:25** Panelist 2 - Judith Giordan, CaN co-Founder & Managing Director ecosVC

**3:40** Panelist 3 - Hugh James, CaN Member & CEO, PCG Inc.

**3:55** Panelist 4 - Catherine Mott, Founder, Managing Partner, BlueTree Venture Fund & BlueTree Allied Angels

**4:10 Paper 7d:** Company Pitch #1

**4:45 Paper 7e:** Company Pitch #2

**5:20 Paper 7f:** Company Pitch #3

**5:50** Concluding Remarks

### (8) Public Affairs and AIChE: A PAIC Town Hall

**Sunday, Oct 28, 3:00 PM**

David L. Lawrence Convention Center, 307

**Nada Marie Anid, Chair**

**Sponsored by:** Public Affairs and Information Committee (PAIC)

**3:00** Welcoming Remarks

**3:05** Climate Change Adaptation and Resilience Task Force Chair: Mary Ellen Ternes

**3:20** Advanced Manufacturing Task Force Chair: Mike Malone

**3:35** Deregulatory Actions: Mary Ellen Ternes

**3:50** Open Discussion and Policy Priorities for 2019 and Beyond

### (9) 3D Printing I

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 333

**Kuo Chen Tsai, Chair**  
**Azita Ahmadzadeh, Co-Chair**

**Sponsored by:** 3D Printing

**3:30** Break

**3:50 Paper 9b:** Development of Nanoparticle Alignment Regimes in Drying Cellulose Nanocrystal Droplet Suspensions for Additive Manufacturing — *Michael J. Bortner, Cailean Pritchard, Maren Roman*

**4:10 Paper 9c:** Characterization of Poly(ether imide) Towards the Development of a Fused Filament Fabrication (FFF) Process Model — *Eric L. Gilmer, Craig D. Mansfield, Donald G. Baird, Michael J. Bortner*

**4:30 Paper 9d:** Additive Manufacturing of Core-Shell Microparticles Containing Thermosetting Resins — *Guozhen Yang, Mengfei Huang, John Klier, Jessica D. Schiffman*

**4:50 Paper 9e:** Supersonic-Impaction Printing of Flame-Made Doped-Perovskite Nanoparticles — *Souvik Ghosh, Eirini Goudeli, Chenxi Li, Bernard Olson, Christopher J. Hogan Jr.*

**5:10 Paper 9f:** Simulating Powder Handling Processes in Additive Manufacturing Using the Discrete Element Method — *David Curry, Carles Bosch Padros*

### (10) Accelerated Discovery and Development of Inorganic Materials

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 329

**Sankar Nair, Chair**  
**Dongxia Liu, Co-Chair**  
**Basudeb Saha, Co-Chair**

**Sponsored by:** Inorganic Materials

**3:30** Break

**3:51 Paper 10b:** A Database of 2D Zeolite Nanosheets: Development and Applications in High Throughput Separations Screening — *Omar Knio, Apar Shanker, Sankar Nair, David S. Sholl*

**4:12 Paper 10c:** Cutting Materials in Half: A Graph Theory Approach for Generating Crystal Surfaces and Its Prediction of Two-Dimensional Zeolites — *Matthew Witman, Sanliang Ling, Peter Boyd, Senja Barthel, Maciej Haranczyk, Ben Slater, Berend Smit*

**4:33 Paper 10d:** Speeding up the Synthesis of Zeolites: From Several Days to Several Seconds — *Zhendong Liu, Jie Zhu, Toru Wakihara, Tatsuya Okubo*

**4:54 Paper 10e:** New Tolerance Factor to Predict the Stability of Perovskite Oxides and Halides — *Christopher J. Bartel, Christopher Sutton, Bryan Goldsmith, Runhai Ouyang, Charles B. Musgrave, Luca M. Ghiringhelli, Matthias Scheffler*

**5:15 Paper 10f:** Creating a Redox Materials Database for Solar-Thermochemical Processes — *Josua Vieten, Patrick Huck, Dorottya Guban, Matthew Horton, Brendan Bulfin, Martin Roeb, Kristin Persson, Christian Sattler*

**5:36 Paper 10g:** Development of a Bond-Centric Model for Thermodynamic Stability of Nanoalloys — *Michael G. Taylor, Zihao Yan, Ashley Mascareno, Giannis Mpourmpakis*

### (11) Advanced Materials for Carbon Dioxide Capture for Power Generation

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 321

**David Hopkinson, Chair**  
**Zachary Smith, Co-Chair**

**Sponsored by:** Advances in Fossil Energy R&D

**3:30 Paper 11a:** Fabrication and Field Testing of Spiral-Wound Membrane Modules for CO<sub>2</sub> Capture from Flue Gas — *Witopo Salim, Varun Vakharia, Yuanxin Chen, Dongzhu Wu, Yang Han, W.S. Winston Ho*

**3:49 Paper 11b:** Low Viscosity Water-Lean Diamine Solvents for Carbon Dioxide Capture — *Phillip K. Koeh, Deepika Malhotra, Manh Nguyen, David J. Heldebrandt, Andy J. Zwoster, Vassiliki-Alexandra Glezakou, Feng Zheng, Roger Rousseau*

**4:08 Paper 11c:** High Swing Capacity MIL-101(Cr) Fiber Sorbents for Sub-Ambient CO<sub>2</sub> Capture Via RCPA — *Stephen J.A. DeWitt, Rohan Awati, Matthew Realff, David S. Sholl, Ryan Lively*

**4:27 Paper 11d:** Carbon Dioxide Capture By an Electrochemically-Mediated Amine Regeneration — *Mohammad Rahimi, Miao Wang, Subrahmaniam Hariharan, Michael Massen-Hane, T. Alan Hatton*

**4:46 Paper 11e:** Layer-By-Layer Functional Thin Film Coatings for Enhanced Light Gas Separations — *Benjamin Wilhite, Jaime C. Grunlan*

**5:05 Paper 11f:** Facilitated Transport Membranes for Hydrogen Purification from Coal-Derived Syngas — *Yang Han, W.S. Winston Ho*

**5:24 Paper 11g:** Novel Membranes for CO<sub>2</sub> concentration and Carbon Capture — *Ning Shangquan, Kenneth J. Pennisi*

**5:43 Paper 11h:** Process Development of Novel Sub-Ambient Membrane Processes for CO<sub>2</sub> Capture — *Jin-Kuk Kim, Sunghoon Lee, Seokwon Yun*



**Celebrating 110 Years**  
**of AIChE, Chemical Engineering**  
**and You, our Members!**

**(12) Advanced Oxidation Processes****Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 319

Selma Mededovic Thagard, Chair  
Tapas Das, Co-Chair**Sponsored by:** Water**3:30 Paper 12a:** Advanced Oxidation Processes for the Treatment of Azole-Containing Industrial Wastewater— *Rui Li, Dinusha Siriwardena, Thomas Holsen, Selma Mededovic Thagard***3:50 Paper 12b:** Cavitation and Immobilised Photo-Catalysis for Effluent Treatment: A Comparative Study of Individual and Combined Operations — *Sebastien J. De-Nasri***4:10 Paper 12c:** Degradation of Acesulfame Potassium By Ferrate(VI) and HCl-Activated Ferrate(VI) in Aqueous Solution — *Malini Ghosh, Kyriakos Manoli, Virender K. Sharma, Ajay K. Ray***4:30 Paper 12d:** Advanced Oxidative Degradation of Benzoic Acid and 4-Hydroxy Benzoic Acid in Aqueous Phase – a Comparative Study — *Bhavna D Deshpande***4:50 Paper 12e:** AOP Performance at Wastewater Treatment Plants — *Jason A. Heberling, Yusuf G. Adewuyi, Ahmed S. Mahmoud, Mohamed K. Mostafa, Dr. Robert W. Peters***5:10 Paper 12f:** A Multi-Dimensional Strategy for Treatment of Raw Landfill Leachate Wastewater Using Electroperoxone — *Ramya Srinivasan, Indumathi Nambi***5:30 Paper 12g:** Aqueous Organics Degradation in Visible Light and Ozone Integrated Process with WO<sub>3</sub> catalysts — *Yongbing Xie, Jin Yang, Honbin Cao***5:50 Paper 12h:** Application of Advanced Oxidation Process for the Treatment of Hydrocracked Water — *Shikha Sinha, Debashis Roy, Sudarsan Neogi, Sirshendu De***(13) Applications of Molecular Modeling to Study Interfacial Phenomena I****Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 308

Vance Jaeger, Chair  
Harold W. Hatch, Co-Chair**Sponsored by:** Computational Molecular Science and Engineering Forum**3:30 Paper 13a:** Understanding Confinement Effects in Mixed Ionic Liquid Systems: Insights from Molecular Dynamics Simulations — *Matt Thompson, Yury Gogotsi, Katherine L. Van Aken, Peter T. Cummings***3:45 Paper 13b:** Modulating the Self-Assembly of 1-n-Dodecyl-3-Methylimidazolium Octylsulfate Bimphiphilic Ionic Liquid — *Utkarsh Kapoor, Jindal K. Shah***4:00 Paper 13c:** Probing Surfactant-Nanoparticle Interactions at Fluid-Fluid Interfaces — *Ashwin Kumar Yegya Raman, Amir Erfani, Jindal K. Shah, Clint P. Aichele***4:15 Paper 13d:** Force Field Parameters for Hydrogen, Oxygen, and Nitrogen to Study Complex Phase Equilibria and Interfacial Reactions — *Shiyi Wang, Hendrik Heinz***4:30 Paper 13e:** Investigating the Effect of Concentration on the Interaction of Electrolytes with Interfaces — *Arushi Prakash, Christopher Fu, Kayla Sprenger, Christopher J. Mundy, Jim Pfendtner***4:45 Paper 13f:** Screening Structure-Property Relationships in Lubricating Monolayer Films through Molecular Dynamics Simulation — *Andrew Z. Summers, Christopher R. Iacovella, Peter T. Cummings, Clare McCabe***5:00 Paper 13g:** Surface Diffusion of Large Molecules: A Computational Study — *Kutay Berk Sezginel, Christopher E. Wilmer***5:15 Paper 13h:** Meso-Scale Modeling of PNIPAM Brushes — *Kartek K. Bejagam, Yixin An, Samrendra Singh, Sanket A. Deshmukh***5:30 Paper 13i:** Molecular Simulation of Ionic Polyimides and Ionic Liquid Composite Membranes for Gas Selectivity and Adsorption — *Asghar Abedini, Joanna Szala-Bilnik, Ellis Crabtree, Jason E. Bara, C. Heath Turner***5:45 Paper 13j:** Hierarchical Multiscale Simulations of Polymeric Nanostructured Materials — *Vagelis A. Harmandaris, Anastassia N. Rissanou, Petra Bačová***(14) Applied Environmental Catalysis****Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 403

Di Wang, Chair  
Erdem Sasmaz, Co-Chair  
Changsheng Su, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**3:30 Paper 14a:** Low Temperature NO and Hydrocarbon Trapping over Pd-Exchanged Zeolite Passive NOx Adsorbers — *Sam Malamis, Michael Harold***3:50 Paper 14b:** Ion-Exchanged Zeolites for Hydrocarbon Traps and Passive NO<sub>x</sub> Adsorption Applications — *Jungkuk Lee, Vivek Vattipalli, Wei Fan, Eleni A. Kyriakidou***4:05 Paper 14c:** Excellent Hydrothermal Stability of Composite Catalyst Based on Two Cu-CHA Type Molecular Sieves — *Yuhan Ma, Yongdan Li***4:20 Paper 14d:** Effects of Surface Species and Dispersion of CeO<sub>2</sub> Supported Transition Metal Oxide Catalysts for NO Reduction By CO Reaction — *Shuhao Zhang, Taejin Kim***4:35 Paper 14e:** Fast Lean-Rich Cycling for Enhanced NO<sub>x</sub> Conversion on Pt/CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> — *Zhiyu Zhou, Michael Harold, Dan Luss***4:50 Paper 14f:** Degrading Organic Compounds in Simulated Produced Water By Creating Hydroxyl Radicals Catalytically — *Yiyuan Yin, Kimberly N. Heck, Camilah Powell, Christian L. Coonrod, Sujin Guo, Michael S. Wong***5:05 Paper 14g:** Swellable Organically Modified Silica (SOMS): A Novel Support for Pd Catalyzed Hydrodechlorination of Trichloroethylene in Aqueous Phase — *Gokhan Celik, Saurabh Ailawar, Seval Gunduz, Jeffrey T. Miller, Franklin (Feng) Tao, Paul Edmiston, Umit S. Ozkan***5:20 Paper 14h:** Treatment of OIL Produced Water Using Advanced Oxidative Processes: Heterogeneous-Photocatalysis and Photo-Fenton — *Priscila C. Silva, Nathalia P. Ferraz, Elen A. Perpetuo, Yvan J. O. Asencios***5:35 Paper 14i:** Electrochemical Anthraquinone Process Enabled By Phase Transfer Catalysis — *Sahag Voskian, Alexander T. Murray, Yogesh Surendranath, T. Alan Hatton***(15) Automation and High-Throughput Technologies for Pharmaceutical Discovery and Development****Sunday, Oct 28, 3:30 PM**

Westin Convention Center, Fayette

Brandon Reizman, Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum**3:30 Paper 15a:** A New High-Throughput Assay for Quantification of Antibiotic Penetration in Gram-Negative Bacterial Cells — *Huan Gu, Zhaowei Jiang, Dacheng Ren***3:50 Paper 15b:** Deploying Automation to Execute Real-Time Feed Strategies in Bench-Scale Bioreactor Systems — *Kristin O'Neill, William Tran, Linda Hoshan, Sen Xu, T. Craig Seamans***4:10 Paper 15c:** Very Large Scale Microfluidic Droplet Integration for Continuous Industrial Scale Manufacturing of Monodisperse Biodegradable Micro and Nanoparticles — *Sagar Yadavali, Heon Ho Jeong, Daeyeon Lee, David Issadore***4:30 Paper 15d:** Applying Automation and Data-Driven Modeling to Perform Rapid Reaction Optimization — *Daniel Griffin, Seth Huggins***4:50 Paper 15e:** Piezoelectric-Based Spray Solvent Delivery System for Desorption Electrospray Ionization Mass Spectrometry: Design & Case Studies for High Throughput Reaction Screening — *Botond Szilagyi, Andy Koswara, Bradley P. Loren, Harrison S. Ewan, Christina E. Ferreira, David H. Thompson, Robert G. Cooks, Zoltan K. Nagy***5:10 Paper 15f:** Closed-Loop Reaction Optimization in Microscale Oscillating Droplets: An MINLP Algorithm Applied to Suzuki-Miyaura Coupling Catalyst Selection — *Connor W. Coley, Lorenz M. Baumgartner, Brandon Reizman, Kevin W. Gao, Klavs F. Jensen***5:30 Paper 15g:** Reaction Screening in an Automated Droplet Screening System for Pharmaceutical Process Development — *Michael Wlekinski, Brandon Reizman*



## (16) Biobased Intermediates and Biomaterials

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 335

Yihui Tom Xu, Chair  
Shaibal Roy, Co-Chair

**Sponsored by:** Process Research and Innovation

**3:30 Paper 16a:** Effects of Solvent Selection on Efficient Furfural Production — **Jacob Dickinson, Torren Carlson, David W. Drew, Paul Fagan, Keith Hutchenson, Gregg Sunshine**

**3:55 Paper 16b:** Synthesis & Characterization of Molecularly Hybrid Bisphenols Derived from Lignin & Cashew Nutshell Liquid: Resin and Polymer Properties — **Kayla R. Sweet**

**4:20 Paper 16c:** The Future in Date Palm Biomass: Characterization of Leaflet, Rachis and Fibers of Lignocellulosic Date Palm Biomass for Future Production of High Value Chemicals — **Emmanuel Galiwango**

**4:45 Paper 16d:** Synthesis, Design and Thermodynamic Analysis of Hybrid Processes Gasifying Biomass and Smelting Iron — **Neil Thomas Stacey, Baraka Celestin Sempuga, Mpendulo Ncongwane**

**5:10 Paper 16e:** F D M E (2,5-Furandicarboxylate, DiMethyl Ester) Process Development: Scale-up through Pilot — **Stuart Fergusson, April Hoffart, Stephen Howard, Keith Hutchenson**

**5:35 Paper 16f:** Reuse and Valorization of Used Cooking Oils By Transformation into Epoxidized Oils — **Luz Angela Rincón Vija, Juan Guillermo Cadavid, Alvaro Orjuela**

## (17) Biobased Materials: Design and Application

**Sunday, Oct 28, 3:30 PM**

Westin Convention Center, Westmoreland West-Central

Phanourios Tamamis, Chair  
Ian Wheeldon, Co-Chair

**Sponsored by:** Bioengineering

**3:30 Paper 17a:** Determining the Role of Peptide Nanocluster Characteristics on Dendritic Cell Antigen Processing in Peptide Vaccines — **Alexandra Tsoras, Julie A. Champion**

**3:48 Paper 17b:** Evaluation of Catechol Use As a Crosslinker and to Functionalize Chitosan to Produce a Bone Adhesive with Aqueous Adhesion — **Paula A Sarmiento, J. German Vargas, Felipe Salcedo**

**4:06 Paper 17c:** Structure-Function-Dynamics Relationships in Next Generation Protein-Polymer Conjugates — **Stefanie Baker, Aravinda Munasinghe, Hironobu Murata, Krzysztof Matyjaszewski, Ping Lin, Coray M. Colina, Alan Russell**

**4:24 Paper 17d:** Short Elastin-like Peptides Engineered to Control Ionomer on Metal Surfaces for Electrode Manufacturing Applications — **Zihang Su, Nuttanit Pramounmat, Skylar Watson, Julie N. Renner**

**4:42 Paper 17e:** Biocompatible Genetically-Engineered Outer Membrane Vesicles with Expressed Nanoluc Reporter: Preparation, Characterization and *In Vivo* Kinetic Modeling — **Yikun Huang, Andre Beringhs, Qi Chen, Mu-Ping Nieh, Xiuling Lu, Tai-Hsi Fan, Wilfred Chen, Yu Lei**

**5:00 Paper 17f:** Creating Proteins with Large Sizes and New Shapes for Biomedical Applications — **Kevin Metcalf, Milan Mrksich**

**5:18 Paper 17g:** Employing Bacterial Secretion for a High-Throughput Biomaterials Production and Screening Platform — **Danielle Tullman-Ercek**

## (18) Bioinspired Membranes and Membrane Processes

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 302

Zhongyi Jiang, Chair  
Manish Kumar, Co-Chair  
Ronald Michalsky, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 18a:** Bioinspired Membranes for CO<sub>2</sub> Capture — **Zhongyi Jiang**

**3:49 Paper 18b:** Spray-Coated Multilayer Cellulose Nanocrystal – Chitin Nanofiber Films for Barrier Applications — **Chinmay C. Satam, Cameron Irvin, Augustus Lang, Jerel Jallorina, Meisha Shofner, John Reynolds, Carson Meredith**

**4:08 Paper 18c:** Fe(III)-Induced Polydopamine Coating with “Deposition-Polymerization” Mechanism for Microfiltration Membrane Hydrophilization — **Xuehua Ruan, Xuhang Liao, Gaohong He, Yan Dai, Xiaobin Jiang**

**4:27 Paper 18d:** Creating Biomimetic Membranes with Uniform Subnanometer Pore By Co-Assembly of Well-Oriented Lamellar Block Copolymer with Artificial Channels — **Chao Lang, Dan Ye, Woonchul Song, Jacob A. LaNasa, Yuexiao Shen, Robert J. Hickey, Manish Kumar**

**4:46 Paper 18e:** Bio-Inspired Membrane Based Self-Organizing System — **Hiroshi Umakoshi, Keishi Suga**

**5:05 Paper 18f:** Performance Evaluation of Novel Nano-Structured Modified Mesoporous Silica/Polyetherimide Composite Membranes for the Treatment of Oil/Water Emulsion — **Geethanzali Kamalanathan**

**5:24 Paper 18g:** Bioinspired Biodegradable Superhydrophobic Membrane for Oil-Water Separation Using 3D Printing Technology — **Ruizhe Xing, Wei Qi**

**5:43 Paper 18h:** Design, Synthesis, and Characterization of Artificial Water Channel Based Polymeric Membranes — **Woonchul Song, Yuexiao Shen, Tingwei Ren, Manish Kumar**

## (19) Biomaterials for *in vitro* Tissue Models and Improved Therapeutic Strategies

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 331

Shreyas Rao, Co-Chair  
Steven R. Calia, Co-Chair

**Sponsored by:** Biomaterials

**3:30 Paper 19a:** A Model of Oxidation Injury and an Antioxidant Drug Delivery Rescue Strategy — **Nicholas Murphy, Kyle Lampe**

**3:48 Paper 19b:** A Three-Dimensional Hyaluronic Acid Hydrogel Platform to Study the Mechanobiology and Invasion of Brain Metastatic Breast Cancer Cells — **Akshay Narkhede, James Crenshaw, Riley Manning, Shreyas Rao**

**4:06 Paper 19c:** An *In Vitro* Chondro-Osteo-Vascular Triphasic Model of the Osteochondral Complex — **Riccardo Gottardi, Alessandro Piroso, Peter Alexander, Dario Puppi, Federica Chiellini, Rocky Tuan**

**4:24 Paper 19d:** Investigating the Mechanical Microenvironment on Fibrogenesis in Multi-Cellular Hepatic Models — **Sophia Orbach, Andrew Ford, Scott-Eugene Saverot, Padmavathy Rajagopalan**

**4:42 Paper 19e:** Tissue Guided Design of a Brain ECM Mimicking Hydrogel — **Sualyneth Galarza, Shelly Peyton**

**5:00 Paper 19f:** Culturing the Co-Encapsulated Primary Hepatocytes with Mesenchymal Stem Cells: Study on Effect of Co-Encapsulation and Perfusion on Hepatocyte Metabolic Activity — **Amin Vossoughi Shahvari, Howard W. T. Matthew**

**5:18 Paper 19g:** Mechanical Regulation of Cancer Cell Angiogenic Activity — **Malak Nasser, Gargi Ghosh**

**5:36 Paper 19h:** Layer-By-Layer Assemblies of Collagen/Heparin Towards the Manufacturing of Human Mesenchymal Stem Cells — **David Castilla, José R. Garcia, Wilbur A Lam, Andres Garcia, Jorge Almodovar**

## (20) Bioplastics, Biocomposites and Value-Added Uses of Biofuel Coproducts for Sustainable Manufacturing

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 325

Amar K. Mohanty, Chair  
Manju Misra, Co-Chair

**Sponsored by:** Forest and Plant Bioproducts Division

**3:30 Paper 20a:** Ultrapure Lignin Via the ALPHA Process for Materials Applications: From Carbon Fibers to Coatings — **Mark C. Thies, Junhuan Ding, Jing Jin, Amod Ogale**

**3:55 Paper 20b:** Mixture-Process Variable Experimental Design to Optimize Sugar Mixture (glucose, xylose and arabinose) Conversion to Polyhydroxybutyrate By *Burkholderia Saccharia* — **Mengxing Li, Mark R. Wilkins, Kent Eskridge**

**4:20 Paper 20c:** Integrating Sustainable Biocarbon in Lightweight and Durable Biocomposite Solutions for Automotive Applications — **Amar K. Mohanty, Andrew Anstey, Amandine Codou, Manju Misra**

**4:45 Paper 20d:** Nano-Engineered Cement Combining Biomass Ash with Nanoparticles — **Joan G. Lynam, Narendra Kumar, Kunal Kupwade-Patil, Rayna Higuchi, David P. Ferrell, Vanya A. Luttrull, Oral Buyukozturk**

**5:10 Paper 20e:** A Study on the Gelation Kinetics and Chain Relaxation of Polybutylene Succinate (PBS) By Reactive Extrusion — **Feng Wu, Manju Misra, Amar K. Mohanty**

**5:35 Paper 20f:** Chicken Feather Biocarbon Based Novel Biodegradable Composites — *Zonglin Li, Christoff Reimer, Amar K. Mohanty, Manju Misra*

**(21) Catalytic Hydrogen Generation**  
**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 405

Brett Loveless, Chair  
Shu Hu, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 21a:** Anatase Nanoparticles from Low Pressure Flame Synthesis for Enhanced Photocatalytic Activity — *Ashley M. Pennington, Fuat E. Celik, Stephen D. Tse*

**3:50 Paper 21b:** Application of Ti-Doped MoO<sub>3</sub> microspheres Prepared By Spray Pyrolysis to Partial Oxidation of *N*-Dodecane — *Qusay Bkour, M. Grant Norton, Su Ha*

**4:10 Paper 21c:** Fundamental Mechanistic Studies of Formic Acid Decomposition on Pd Catalysts — *Saurabh Bhandari, Srinivas Rangarajan, Sha Li, Suyash Singh, Christos Maravelias, James Dumesic, Manos Mavrikakis*

**4:30 Paper 21d:** The Effect of Nickel and Magnesium Loadings on the Activity, Selectivity and Stability for Catalytic Dry Reforming of Biogas Using Pt/Cerium-Zirconium Oxide Catalyst — *Yetunde O. Sokefun, Babu Joseph, John N. Kuhn*

**4:50 Paper 21e:** Intrinsic Kinetics of Steam Methane Reforming on a Thin, Nanostructured and Adherent Ni Coating — *Florent Minette, Michael Lugo, Dean Modroukas, Andrew W. Davis, Rajinder Gill, Marco J. Castaldi, Juray De Wilde*

**5:10 Paper 21f:** Development of Metal-Rich Two-Dimensional Catalysts for Highly Efficient Hydrogen Evolution Reaction — *Alireza Kondori, Chris Coble, Mohammad Asadi*

**5:30 Paper 21g:** Comparison of the Direct and Bifunctional Mechanisms through Steady-State Microkinetic Modeling for Hydrogen Electrocatalysis in Alkaline Media — *Luis Rebollar, Maureen H. Tang*

**(22) Chemical Engineering in Sustainability (YCOST) and Policy (WISE) Award Recipient Talks (Invited Talks)**

**Sunday, Oct 28, 4:15 PM**

David L. Lawrence Convention Center, 307

Victoria Baldwin, Chair

**Sponsored by:** Young Professionals Committee (YPC)

**4:15** Welcoming Remarks

**4:20 Paper 22b:** Rebuilding Energy Infrastructures in Puerto Rico: Microgrids as Socio-Technical Systems — *Christina Chen*

**4:35 Paper 22c:** Democratizing Synthetic Biology: Balancing Biosecurity, Biosafety, and Citizen Science — *Ishaan Dev*

**4:50 Paper 22a:** Recycling of Spent Lithium-Ion Battery: Direct-Recycle-Reuse (DR2) Process — *Trevyn Payne, Zachary Oldenburg, Lucille Nunneley, Sommer Skeps, Lei Pan*

**(23) Chemical Engineers for a World of Good: Bringing Hard and Soft Engineering Skills and Sustainability to Undergraduates**

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 315

Alan Zagoria, Chair  
Laura Ford, Co-Chair  
Christi Patton Luks, Co-Chair

**Sponsored by:** General

**3:30** Introductory Remarks

**3:45 Paper 23a:** Important Hard and Soft Skills Difficult to Teach in the Classroom — *Kelly Barb, Alan Zagoria*

**3:55 Paper 23b:** A Student Perspective: What I Learned from Working on an International Project — *George Garner, Donny Gross, Kathryn Lundgren*

**4:20 Paper 23c:** What Does Sustainability Really Mean in These Projects? — *Christi Patton Luks*

**4:30 Paper 23d:** What Is EWB-USA and Why Might You Want to Work with Them? — *Laura Ford*

**4:40 Paper 23e:** How International Projects Might Help with ABET Accreditation — *Randy S. Lewis, Laura Ford*

**4:50 Paper 23f:** Panel Discussion - Making Successful International Projects Happen — *Catherine B. Almquist, Daniel J. Lacks, Randy S. Lewis, John Tharakan*

**5:50** Concluding Remarks

**(24) Dynamic Processes at Interfaces**

**Sunday, Oct 28, 3:30 PM**

Omni William Penn Hotel, Conference Center B

Sepideh Razavi, Chair  
Mark Kastantin, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 24a:** Dynamic Evolution of Drop in Miscible Liquid-Liquid Systems at Low Flow Rate — *Nikhil Joshi, Abhik Majumder, Prasanta Kumar Das*

**3:46 Paper 24b:** Subphase Depth and Surfactant-Driven Marangoni Transport — *Steven Iasella, Timothy Corcoran, Stephen Garoff, Todd Przybycien, Robert D. Tilton*

**4:02 Paper 24c:** Efficient Dispersion of Crude Oil By Food-Grade Surfactants: The Potential of Lecithin — *Geoff Bothun, Vijay T. John, Alon McCormick, Srinivasa R. Raghavan*

**4:18 Paper 24d:** Atomistic Simulations of Micellization and Adsorption of Surfactant Molecules Near Metal-Water Interfaces — *Sumit Sharma, Yathish Kurapati, Himanshu Singh*

**4:34 Paper 24e:** GHz-Dielectric Relaxation Stimulates the Hydration State of Lipid Bilayer Membrane — *Atsushi Tauchi, Yukihiro Okamoto, Keishi Suga, Hiroshi Umakoshi*

**4:50 Paper 24f:** Measuring the Adsorption Dynamics of a Switchable Tertiary Amine Surfactant Using QCM — *Yi-Lin Chen, Sibani Lisa Biswal*

**5:06 Paper 24g:** Magneto-Capillary Dynamics of Amphiphilic Janus Particles at Curved Liquid Interfaces — *Wenjie Fei, Michelle Driscoll, Paul M. Chaikin, Kyle J. M. Bishop*

**5:22 Paper 24h:** Quantifying the Stability of Magnetic Surfactants in Aqueous Solution — *Alex Fortenberry, Derek Reed, Adam E. Smith, Paul Scovazzo*

**5:38 Paper 24i:** Dynamics and Morphological Evolution of Graphene and Graphite Films at Fluid-Fluid Interfaces — *David M. Goggin, Joseph R. Samaniuk*

**(25) Electrochemical Storage Materials and Devices**

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 330

Gang Wu, Chair  
Juchen Guo, Co-Chair  
Vincent C. Holmberg, Co-Chair

**Sponsored by:** Electronics and Photonics

**3:30 Paper 25a:** *Invited:* Versatile Redox-Active Organic Molecules for Long Cycle Life Safe Batteries — *Yan Yao*

**3:55 Paper 25b:** *Invited:* Exploring Electrochemical Reaction Dynamics of Li+-Solvation Structures with Large-Scale Quantum Mechanical Simulations — *Bryan M. Wong, Juchen Guo, Chengyin Fu, Lihua Xu, Fredy W. Aquino*

**4:20 Paper 25c:** *Invited:* Novel Materials and Modification of Lithium Sulfur Batteries of Enhanced Performance — *Simon Ng, Wenduo Zeng, Mark Cheng*

**4:40 Paper 25d:** *Invited:* Charge Storage Mechanisms and Ion Transport in Aluminum-Graphite Batteries — *Robert J. Messinger, Jeffrey Xu, Damon Turney*

**5:00 Paper 25e:** New Figure of Merit for Nano-Rectenna Based THz Energy Harvesters — *Patrick J. Pinhero, Evan Allison*

**5:20 Paper 25f:** Magnesium Deposition from Sulfone-Ether Electrolytes — *Laura Merrill, Jennifer Schaefer*

**5:40 Paper 25g:** The Effect of Electrochemical Lithium Insertion on the Electronic Conductivity of TiO<sub>2</sub> (anatase) and Its Application in Neuromorphic Computing — *Yiyang Li, Elliot J. Fuller, Sapan Agarwal, A. Alec Talin*

**(26) Engineering in Development and Aging**

**Sunday, Oct 28, 3:30 PM**

Westin Convention Center, Butler

Jeremiah J. Zartman, Co-Chair  
David M. Umulis, Co-Chair  
Kris Noel Dahl, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**3:30 Paper 26a:** An Auto-Catalytic Cell Intercalation Mechanism to Understand Tissue Elongation during Morphogenesis — *Samira Anbari, Javier Buceta*

**3:48 Paper 26b:** Dynamic Control of Gene Expression in Developing Embryos — **Bomyi Lim, Takashi Fukaya, Michael Levine**

**4:06 Paper 26c:** Measuring Changes in Cell Mechanics and Nuclear Rheology Associated with Cellular Transitions in Monolayers Associated with Development — **Kirill Lavrenyuk, Travis Armiger, Paul Arsenovic, Kranthidhar Bathula, Daniel Conway, Kris Noel Dahl**

**4:24 Paper 26d:** Metabolic Network Analysis for Understanding the Biology of Aging — **Sudharsan Ravi, Rudiyanto Gunawan**

**4:42 Paper 26e:** Microfluidic Device for Life-Long High-Resolution and High-Throughput Imaging of Subtle Phenotypes in *C. Elegans* — **Sahand Saberi Bosari, Adriana San-Miguel**

**5:00 Paper 26f:** Stochastic Analysis of Information Transduction Via BMP Receptor Oligomerization during Embryogenesis — **Aasakiran Madamanchi, Mohammad Shahriar Karim, David M. Umulis**

**5:18 Paper 26g:** Invited Speaker: Quantitative Models of Cell-Cell Signaling in Development — **Greg Reeves**

#### (27) Feedstock Logistics for Biorefineries

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 316

Vicki S. Thompson, Chair  
Chang Dou, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**3:30 Paper 27a:** Controlling Particle Size in 2 Stage Grinding Processes — **Neal Yancey, Matthew Anderson, Craig Conner, Jaya Shankar Tumuluru**

**3:55 Paper 27b:** Impact of Parcel Size, Field Shape, Crop Yield, Storage Location and Collection Equipment on the Performance of Harvest System in Shrub Willow Fields — **Mahmood Ebadiana, Magen Elizabeth Sheddenb, Erin Webb, Shahab Sokhansanj, Mark Eisenbies, Timothy A. Volk, Justin Heavey, Karl Hallen**

**4:20 Paper 27c:** Investigating the Distributed and Centralized Preprocessing Depot in the Supply Chain Network Design of a Biorefinery Designed for Biochemical Conversion — **Roni Mohammad, Damon Hartley, David N. Thompson**

**4:45 Paper 27d:** Willow Biomass As a Feedstock for Biorefinery: Evaluation of Bark Effect on Hot Water Extraction Output, and Lifecycle Assessment of Cellulosic Ethanol Production — **Obste Therasme, Timothy A. Volk, Thomas Amidon, Marie-Odile Fortier**

**5:10 Paper 27e:** Techno-Economic Analysis of Supplying Forest Biomass Feedstock for Biopower Applications — **HakSoo Ha, Ryan J. Quinn, Tristan Brown, Marie-Odile Fortier, Timothy A. Volk, Jenny Frank, Robert Malmshheimer**

**5:35 Paper 27f:** Performance and Logistics of a Forage Harvester and Collection System in Short Rotation Willow Crops — **Mark Eisenbies, Timothy A. Volk, Daniel P. De Souza, Obste Therasme, Karl Hallen**

#### (28) Fuel Cell Membranes

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 303

W.S. Winston Ho, Co-Chair  
Peter N. Pintauro, Co-Chair  
He Bai, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 28a:** Design and Development of Advanced Automotive Fuel Cell Membranes — **Ruichun Jiang, Craig Gittleman**

**3:51 Paper 28b:** Design of 2-D Novel Materials for Anhydrous Proton Transport — **Abhishek Bagusetty, J. Karl Johnson**

**4:12 Paper 28c:** Quantitative Structure Analysis of Polymerized Ionic Liquids with Atomistic Molecular Simulations — **Stephen Paddison**

**4:33 Paper 28d:** Saturated *N*-Heterocyclic Cationic Polymers As Anion Exchange Membranes in Alkaline Fuel Cells — **Rui Sun, Monica Hwang, Carl L. Willis, Yossef A. Elabd**

**4:54 Paper 28e:** Highly Durable Direct Formate Solid Alkaline Fuel Cells Using New Aromatic Anion Exchange Polymer and Carbon Free Electro-Catalysts — **Takeo Yamaguchi, Shoji Miyaniishi, Ayaka Sakakibara, Takanori Tamaki, Sanker Sasidharan, Gopinathan M. Anilkumar**

**5:15 Paper 28f:** Oxidatively Stable Borate-Containing Membranes for H<sub>2</sub> Purification for Fuel Cells — **Witopo Salim, Varun Vakharia, Kai Chen, Michael Gasda, W.S. Winston Ho**

**5:36 Paper 28g:** Free Volume Enhanced Ion Transport in Anion Exchange Membranes for Fuel Cell Application — **Kuibo Zhang, Baoqiang Zhang, Shoutao Gong, Fengxiang Zhang**

**(29) Fuels from the Sun: Nanomaterials for Water Splitting, Artificial Photosynthesis, and Other Photocatalytic and Photoelectrochemical Reactions**  
**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 412

Jinwoo Lee, Chair

**Sponsored by:** Nanomaterials for Applications in Energy and Biology

**3:30 Paper 29a:** Selectivity of Photocatalytic Conversion of Carbon Dioxide Modulated By Surface Ligands on Cu<sub>2</sub>O/TiO<sub>2</sub> Particles — **Doh C. Lee**

**4:00 Paper 29b:** Oxygen-Deficient Monoclinic Tungsten Oxide Nanowires for Spectrally Selective Electrochromic Smart Windows — **Shengliang Zhang, Sheng Cao, Tianran Zhang, Qiaofeng Yao, Adrian C. Fisher, Jim Yang Lee**

**4:30 Paper 29c:** Solar-Driven Photocatalytic Reforming of Glycerol for Hydrogen Production over Ternary Cu/TiO<sub>2</sub>/Graphene Photocatalyst: Effects of Reaction Conditions — **Tumelo W.P. Seadira, Thabang Ntho, Cornelius Mduduzi Masuku, Michael S. Scurrall**

**4:49 Paper 29d:** Structural Effect Study in an Assembled Nano-Heterojunction Towards Designing a Visible Light Photocatalyst for H<sub>2</sub> Generation — **Md Moniruddin, Branden Meusling, Abubacarr Kaira, Abel Abraham, Nurxat Nuraje**

**5:08 Paper 29e:** Cooperative Effect of Co and Zr Co-Doping on the Photoelectrochemical Water Splitting Performance of Hematite — **Qiyang Huang, Yongdan Li**

**5:27 Paper 29f:** Incorporation of Photosystem 1 in Three-Dimensional High Surface Area Electrodes — **Faustin Mwambutsa, Andrew Naclerio, Piran Kidambi, David Cliffler, G. Kane Jennings**

**5:46 Paper 29g:** Photo-Catalytic Degradation of Pharmaceuticals in Water Matrix Under Simulated Solar Light Using BiOCl/BiOI — **Ukoha Emekwo, A. G. Agwu Nnanna, John D. Vargo, Nicholas Baumhover**

#### (30) Fundamentals of Food, Energy, and Water Systems

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 320

Urmila M. Diwekar, Chair  
JoAnn S. Lighty, Co-Chair

**Sponsored by:** Fundamentals

**3:30 Paper 30a:** Pittsburgh: Urban Agriculture and the Nexus — **Thomas Tarka**

**3:51 Paper 30b:** Quantifying Virtual Phosphorus Flows in Interstate Food Trade: Implications for Environmental Sustainability — **Nemi Vora, Elaine M Yates, Vikas Khanna**

**4:12 Paper 30c:** Towards a Two-Level Superstructure Optimization Framework for Land Use Based on Food-Energy-Water Nexus — **Yaling Nie, Styliani Avraamidou, Jie Li, Xin Xiao, Stratos Pistikopoulos**

**4:33 Paper 30d:** Land Availability, Utilization, and Intensification for a Solar Powered Economy — **Yiru Li, Rakesh Agrawal**

**4:54 Paper 30e:** Microbial Community Profile Versus Water Quality in Urban Watersheds — **Adrian Low, Matthew J. Rogers, Jianzhong He**

**5:15 Paper 30f:** Mechanisms Whereby Microbes Promote Intermediate Soil Moisture Content — **Yi-Syuan Guo, Jessica M. Furrer, Daniel J. Gage, Yongku Cho, Leslie M. Shor**

**5:36 Paper 30g:** Nitrogen Efficient Fertilizer Materials — **Jonas Baltrusaitis**

#### (31) Green Chemical Reaction Engineering for Sustainability

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 401

Samuel Marre, Chair  
Miguel Modestino, Co-Chair  
Simon Kuhn, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 31a:** Methane (sI) Hydrate Crystallization and Dissociation in a Thermoelectrically-Cooled Microreactor — **WeiQi Chen, Bruno Pinho, Ryan L. Hartman**

**3:50 Paper 31b:** C-H Activation By Ozone in Liquid CO<sub>2</sub> — **Xuhui Chen, Derek Rice, Andrew Danby, Michael D. Lundin, Timothy Jackson, Bala Subramaniam**



**4:10 Paper 31c:** pH Sensitive Colloidal Gold Nanoparticle Catalysts for Enhanced Recovery and Reuse — **Saptarshi Chakraborty**, Christopher L. Kitchens

**4:30 Paper 31d:** CO<sub>2</sub> Conversion Via RWGS-CL over La-Perovskite Oxide with Three Metals (Co, Fe, and Mn) in the B-Site — **Adela E. Ramos**, Debtanu Maiti, Yolanda Daza, J. N. Kuhn, Venkat R. Bhethanabotla

**4:50 Break**

**5:10 Paper 31f:** High Performance Non-Mercury Catalysts for VCM Production: From Theoretical Study to Industrialization — **Hao Xu**, Guohua Luo

**5:30 Paper 31g:** Chloroplast-Inspired Artificial Photosynthetic Capsules for Efficient and Sustainable Enzymatic Hydrogenation — **Jiafu Shi**

### (32) Hybrid Separation Processes

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 301

Joshua A. Thompson, Chair  
Ryan Lively, Co-Chair

**Sponsored by:** General Topics and Other Methods

**3:30 Paper 32a:** A Systematic Approach for Membrane-Based Hybrid Separation Network Synthesis — **Salih E. Demirel**, Jianping Li, M. M. Faruque Hasan

**3:52 Paper 32b:** Immobilised Solvent Systems: Evaluating the Potential of High Surface Area Membrane/Solvent Hybrid Sorbent Materials — **Thomas Moore**, Kathryn A. Mumford, Geoffrey W. Stevens, Paul A. Webley

**4:14 Paper 32c:** A Synthesis Framework for Hybrid Separation Sequences Based on Reduced Directed Graph Superstructure — **Yang Yang**, Xiong Zou, Haotian Ye, Weixuan Zhu, Chongming Gao, Hong-guang Dong

**4:36 Break**

**4:58 Paper 32e:** Kinetic Study of Degradation of Pharmaceutical Drugs By Ozone Microbubbles — **Prof. S. K. Majumder**

**5:20 Paper 32f:** Porous Frozen Material Approach to Freeze-Drying of Instant Coffee — **Wei Wang**, Dapeng Hu, Yanqiu Pan, Qiangqiang Li, Guohua Chen

### (33) Hydrogel Biomaterials

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 328

Mark W. Tibbitt, Co-Chair  
Adam Ekenseair, Co-Chair

**Sponsored by:** Biomaterials

**3:30 Paper 33a:** Logical Breakdown: Encoding Boolean-Based Degradative Responsiveness into Hydrogel Biomaterials — **Barry A. Badeau**, Michael P. Comerford, Christopher K. Arakawa, Jared A. Shadish, Cole A. DeForest

**3:48 Paper 33b:** Force-Responsive, Cryptic Hydrogels to Sense and Respond to Cell Traction — **Yen Tran**, Matthew Rasmuson, Todd Emrick, John Klier, Shelly Peyton

**4:06 Paper 33c:** Reversible Control of Hydrogel Mechanics with Irreversible Photo-Mediated Reactions — **Adrianne M. Rosales**, Sebastian Vega, Frank Del Rio, Jason A. Burdick, Kristi S. Anseth

**4:24 Paper 33d:** Scalable and Tunable Synthetic Hydrogels for Use in Biomaterials Applications — **Owen S. Fenton**, Jason L. Andresen, Marion Paolini, Robert Langer

**4:42 Paper 33e:** Engineering an Adhesive Hydrogel for Corneal Sealing and Regeneration — **Ehsan Shirzaei Sani**, Ahmad Kheirkhah, Devyesh Rana, William Foulsham, Amir Sheikh, Afsaneh Amouzgar, Ali Khademhosseini, Reza Dana, Nasim Annabi

**5:00 Paper 33f:** Injectable Supramolecular Hydrogels with Quasi-Covalent Crosslinking — **Matthew Webber**

**5:18 Paper 33g:** Covalent Adaptable Hydrogel Networks for Delivery during Digestion — **Nan Wu**, Kelly M. Schultz

**5:36 Paper 33h:** Environmentally Responsive Methacrylated Alginate Hydrogel Gradients for Studying NIH/3T3 Fibroblasts — **Anuraag Boddupalli**, Kaitlin Bratlie

### (34) Innovations in Pharmaceutical Discovery, Development, and Manufacturing

**Sunday, Oct 28, 3:30 PM**

Westin Convention Center, Washington

Jonathan P. McMullen, Chair  
Christopher H. Marton, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 34a:** Rational Design of Peptide Nucleic Acid Antibiotics Against Multidrug Resistant Bacteria — **Thomas Aunins**, Colleen Courtney, Kristen Eller, Jocelyn Campos, Keesha Erickson, Anushree Chatterjee

**3:51 Paper 34b:** Identifying CQAs of 3D Printed Extended-Release Tablets through the Optimization of Formulation and 3D Geometric Variables — **Alaadin Alayoubi**, Ahmed Zidan, Mohammad Sabir Aqueel, Celia N. Cruz, Muhammad Ashraf

**4:12 Paper 34c:** A Constrained Version of the Dynamic Response Surface Methodology for Challenging Time-Resolved Pharmaceutical Reaction Data — **Yachao Dong**, Christos Georgakis, Jason Mustakis, Joel M. Hawkins, Lu Han, Jonathan P. McMullen, Shane T. Grosser

**4:33 Paper 34d:** Characterizing Protein-Protein Interactions in Highly Concentrated Monoclonal Antibody Solutions Using Small Angle X-Ray Scattering and Molecular Dynamics Simulations — **Amjad Chowdhury**, Barton J. Dear, Jonathan A. Bollinger, Jessica Hung, P. Douglas Godfrin, Maria P. Nieto, Tony Shay, Logan Wilks, Carl Karouta, Thomas M. Truskett, Keith P. Johnston

**4:54 Paper 34e:** A Case Study and Design Considerations for the Robust Removal of Dissolved Hydrogen Chloride — **Shujauddin M. Changi**, Jonas Y. Buser, Matthew C. Embry, Daniel Jarmer, Christopher L. Burcham, Radhe K. Vaid, Adam D. McFarland, Tim Pletcher, Carla Luciani, Kieran Kearney, Nessa Mullane, D Declan Hurley

**5:15 Paper 34f:** Real-Time Monitoring of Drug Concentration in a Dropwise Additive Manufacturing System — **Andrew J. Radcliffe**, Zoltan K. Nagy, Gintaras V. Reklaitis

**5:36 Paper 34g:** Mechanistic Insights into a Process Intensification Strategy in Pharmaceutical Manufacturing — **Kanjakha Pal**, Zoltan K. Nagy

### (35) Membrane Formation

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 304

Yan Wang, Co-Chair  
Neal Chung, Co-Chair  
Lucy Mar Camacho, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 35a:** Unique Properties of Graphene Oxide Membranes for Membrane Distillation Desalination — **Lucy Mar Camacho**, Samuel O Olatunji

**3:48 Paper 35b:** Improved Antifouling Performance of Polysulfone Ultrafiltration Membrane Via Peptoid Molecules — **Neda Mahmoudi**, John Moore II, Grant Harrison, Jamie Hestekin, Shannon L. Servoss

**4:06 Paper 35c:** Fouling Free Hydrophilic Polysulfone Ultrafiltration Membranes — **Mihir K. Purkait**, Randeep Singh

**4:24 Paper 35h:** Facile Fabrication of Sulfonated Polyphenylenesulfone (sPPSU) Membranes with High Separation Performance for Organic Solvent Nanofiltration — **Yingnan Feng**, Martin Weber, Christian Maletzko, Tai-Shung Chung

**4:42 Paper 35e:** Fabricating Polyurethane/Zelite Mixed Matrix Membranes for Pervaporation of Dilute Aqueous Organic Solvents — **I-Min Hsieh**, Mahdi Malmali

**5:00 Paper 592a:** Investigation of the Impacts of Dope Solution Viscosity on Membrane Morphological and Operational Characteristics — **Xiaobo Dong**, Samantha De Jesus, Isabel Escobar

**5:18 Paper 35g:** High Performance Thin-Film Composite Forward Osmosis Membrane with Novel PVDF/PFSA Substrate — **Xuan Zhang**, Yan Wang

### (36) Microbiomes and Metabolomes in Food, Health, and Bioprocessing

**Sunday, Oct 28, 3:30 PM**

Westin Convention Center,

Westmoreland East

S.T. Yang, Chair  
Xin Xin, Co-Chair

**Sponsored by:** Food

**3:30 Paper 36a:** An ESC-Based Test for High Throughput Screening of Embryotoxicity of Drugs and Chemicals — **Fengli Zhang**, Xin Xin, Shang-Tian Yang

**3:48 Paper 36b:** Functional Role of Bacteria Involved in Cocoa Fermentation Processes According to a Metabolic Prediction Using 16S rRNA Reads — **Mauricio E. Pacheco**, Alejandro Caro Quintero, Alejandro Reyes Muñoz, Andrés F. González

**4:06 Paper 36c:** Quantifying the Effect of Minimal Processing on the Kinetics and Antimicrobial Resistance of *Listeria* in Structured Food Model Systems Enriched with Natural Microflora — **Katherine Costello**, Jorge Gutierrez-Merino, Madeleine J. Bussemaker, Maria Baka, Jan Van Impe, Eirini Velliou

**4:24 Paper 36d:** Microdroplet-Enabled Metagenomic Reconstruction of Draft Genomes from the Human Gut Microbiome — **James Tan, Sida (Steven) Wang, Mark A. Burns, Gregory Dick, Xiaoxia (Nina) Lin**

**4:42 Paper 36e:** Microdroplet Cocultivation and Characterization of Vaginal Bacteria in Vaginal Fluid — **Corine Jackman, Xiaoxia (Nina) Lin**

**5:00 Paper 36f:** Probiotics As Viable Antimicrobials Inhibiting Pathogens during Biofilm Formation — **Kuili Fang, Xing Jin, Shweta Shree, Seok Hoon Hong**

**5:18 Paper 36g:** Microbiomes in Food, Health, and Bioprocessing: Advances and Challenges — **Shang-Tian Yang, Meng Lin**

### (37) Multifunctional Composites

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 323

Luyi Sun, Chair  
Zhengtang Luo, Co-Chair  
Holly A. Stretz, Co-Chair

**Sponsored by:** Composites

**3:30 Paper 37a:** Bio-Inspired Multifunctional Stimuli-Responsive Materials — **Songshan Zeng, Rui Li, Dianyun Zhang, Luyi Sun**

**3:46 Paper 37b:** Plasmonic Nanocrystal/Polymer Nanocomposites Thin Films Based Optical Fiber Chemical Sensors — **Ki-Joong Kim, Jeffery Culp, Paul R. Ohodnicki**

**4:02 Paper 37c:** Biomimetic Nanocoatings with Exceptional Mechanical, Barrier, and Flame-Retardant Properties from Large-Scale One-Step Coassembly — **Jingjing Liu**

**4:18 Paper 37d:** Triboluminescent Composites for Engineering Applications — **Zhaofeng Wang**

**4:34 Paper 37e:** Boosting Thermal Conduction Via Filler-Free Technology in Polymer Based Materials with Good Optical Transparency — **Nitin Mehra, Marjan Alsadat Kashfipour, Jiahua Zhu**

**4:50 Paper 37f:** Broadband Light-Responsive Smart Nanocomposites Enabled By Graphene Oxide-Reinforced Shape Memory Polymers — **Peng Jiang, Calen Leverant**

### (38) Nanofabrication and Nanoscale Processing I

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 310

Shohreh Hemmati, Co-Chair  
Jung-Sheng Wu, Co-Chair

**Sponsored by:** Nanoscale Science and Engineering Forum

**3:30 Paper 38a:** Scalable Fabrication of High Performance Microbatteries, Biosensors and Optical Elements Via Nanoimprinting of 3-D Metal Oxide Structures — **James J. Watkins**

**4:00 Paper 38b:** Enhancing the Selectivity of Gas Sensors By Pre-Separation with Membranes or Powder Filters — **Andreas T. Güntner, Jan van den Broek, Sebastian Abegg, Karsten Wegner, Sotiris E. Pratsinis**

**4:30 Paper 38c:** Low-Cost and High-Throughput Synthesis of Copper Nanopowder for Nanofluid Applications — **Nitai Chandra Maji, Jayanta Chakraborty**

**4:45 Paper 38d:** Synthesis and Online Characterization of Metallic Nanoparticles By Spark Ablation — **Maximilian Domaschke, Melanie Schmidt, Wolfgang Peukert**

**5:00 Paper 38e:** Gas Phase Coating of Germanium Nanoparticles with Silicon — **Lukas Wergen, Maximilian Domaschke, Wolfgang Peukert**

**5:15 Break**

**5:30 Paper 38g:** The Geode Process: A Route to the Large-Scale Manufacturing of Functionally-Encoded Nanostructures — **Maritza Mujica, Victor Breedveld, Sven H. Behrens, Michael A. Filler**

**5:45 Paper 38h:** Mass Production of Nanoscale Materials with Uniform Ultralarge Mesopores Via Colloidal Solution Combustion Synthesis — **Albert A. Voskanyan, Kwong-Yu Chan**

### (39) Nanostructured Biomimetic and Biohybrid Materials and Devices

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 311

Markita Landry, Chair  
Esmail Jabbari, Co-Chair

**Sponsored by:** Bionanotechnology

**3:30 Paper 39a:** Invited Speaker: Carbon Nanotube-Based Optical Sensors for Cancer Detection — **Daniel Heller, Ryan Williams, Thomas Galassi, Jackson Harvey, Prakrit Jena, Janki Shah, Hanan Baker, Daniel Roxbury, Gul H. Zerze, Jeetain Mittal, Douglas Levine**

**4:10 Paper 39b:** Spatial Organization of Islet Cells in a Bioscaffold for Long-Term Glucose-Stimulated Insulin Delivery — **Katy N. Olafson, Robert Langer, Daniel G. Anderson**

**4:25 Paper 39c:** Peptide-DNA Hybrid Nanomaterials for Biology and Medicine — **Ronit Freeman**

**4:40 Paper 39d:** Self-Assembled Hybrid Peptide-DNA and Protein-DNA Nanostructures — **Nicholas Stephanopoulos**

**4:55 Paper 39e:** Dynamic Covalent Assembly of Abiotic, Information-Bearing Oligomers — **Timothy F. Scott, Samuel Leguizamon, Megan Dunn, Tao Wei**

**5:10 Paper 39f:** Coffee-Ring Biomaterials As Nanoglues for Laser-Activated Tissue Sealing — **Inam Ridha, Karthik Pushpavanam, Deepanjan Ghosh, Pranvera Gorenca, Jacquelyn Kilbourne, Jeff Heys, Kaushal Rege**

**5:25 Paper 39g:** Micropatterning of Silk Protein-Conductive Polymer Biocomposites for Fabrication of Flexible Devices — **Meng Xu, Ramendra K. Pal, Sayantan Pradhan, Vamsi K. Yadavalli**

**5:40 Paper 39h:** Chitosan / Cellulose Nanocrystals / Calcium Phosphate Hydrogels for Vertebral Compression Fracture Treatment — **Soheila Aliakbarighavimi, Ethan Lungren, Josselet Allison, Yisheng Sun, Trent Faulkner, Ferris Pfeiffer, Christina Goldstein, Caixia Wan, Bret Ulrey**

### (40) Networked, Decentralized, and Distributed Control

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 408

Joseph Sangil Kwon, Chair  
Joseph Scott, Co-Chair

**Sponsored by:** Systems and Process Control

**3:30 Paper 40a:** Optimal Cleaning Scheduling and Control of Heat Exchanger Networks Under Fouling: Problem Formulation and Solution Strategy — **Federico Lozano Santamaria, Sandro Macchietto**

**3:49 Paper 40b:** Control of a Heating, Ventilation and Air Conditioning (HVAC) System Using Decentralized Extremum Seeking — **Judith Ebegbulem, Martin Guay, John M. House, Timothy I. Salsbury**

**4:08 Paper 40c:** Subsystem Decomposition of Process Networks for Simultaneous Distributed State Estimation and Control — **Xunyuan Yin, Jinfeng Liu**

**4:27 Paper 40d:** Distributed Model Predictive Control Based on NLP Sensitivity — **Tianyu Yu, Jun Zhao, Zuhua Xu, Xi Chen, Lorenz T. Biegler**

**4:46 Paper 40e:** Event-Triggered Model-Based Control and Identification of Networked Process Systems — **Amr Zedan, Da Xue, Nael H. El-Farra**

**5:05 Paper 40f:** Coordination of Distributed MPC Systems with Closed-Loop Prediction Approximation in Dynamic Real-Time Optimization (DRT0) — **Hao Li, Christopher L. E. Swartz**

**5:24 Paper 40g:** Data-Based Sequential Design of Decentralized PID Controllers — **Anikesh Kumar, Min-Sen Chiu**

**5:43 Paper 40h:** Distributed Estimation and Nonlinear Model Predictive Control of a Benzene Chlorination Process — **Davood Babaei Pourkargar, Manjiri Moharir, Ali Almansoori, Prodromos Daoutidis**

### (41) Novel Catalytic and Separation Process Based on Ionic Liquids

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 318

Xiangping Zhang, Chair  
Dickson E. Ozokwelu, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**3:30 Break**

**3:51 Paper 41b:** Enhanced CO<sub>2</sub> Electroreduction in Selectivity Tuned By Anion Modification of the Ionic Liquids — **Jianpeng Feng, Shaojuan Zeng, Suojian Zhang, Xiangping Zhang**

**4:12 Paper 41c:** Understanding the Role of Ionic Liquids in the Enzyme Catalyzed Breakdown of Cellulose Using Molecular Dynamics Simulations — **Sarah Alamdari, Jim Pfaendtner**



Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AICHEvents app.



**4:33 Paper 41d:** Novel Ionic Liquids Preparation and Application in Gas Separation Process — **Haifeng Dong, Shaojuan Zeng, Xiangping Zhang, Suojiang Zhang**

**4:54 Paper 41e:** Isobutane Alkylation with C4 Olefin Catalyzed by Combination of SO<sub>3</sub>H-Functionalized Ionic Liquids and Sulfuric Acid — **Weizhong Zheng, Piao Cao, Weizhen Sun, Ling Zhao**

**5:15 Paper 41f:** Superoxide-Derived CO<sub>2</sub> Reduction at Low over-Potentials and Ultra-Fast: A General Approach in Ionic Liquids — **Zhe Wang**

**5:36 Paper 41g:** Biocatalysis in Anhydrous Ionic Liquids — **Jason P. Hallett, Alex Brogan**

**(42) Novel Experimental Methods for the Study of Interfacial Phenomena**  
**Sunday, Oct 28, 3:30 PM**  
Omni William Penn Hotel, Frick

Raymond R. Dagastine, Chair  
Kai Kristiansen, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 42a:** The Design of Two Approaches to Confinement Combined with X-Ray Reflectivity for Structural and Force Studies of Soft Matter at Interfaces — **Laura L. E. Mears, Wiebe M. de Vos, Robert Barker, Stephen Abbott, Robert M. Richardson, Stuart W. Prescott, Pierluigi Bilotto, Max Lengauer, Sadhana Buvaneshwaran, Henning Weiss, Hsiu-Wei Cheng, Claudia Merola, Julian Mars, Markus Mezger, Markus Valtiner**

**3:45 Paper 42b:** Contact Angles in scCO<sub>2</sub>-Brine-Sandstone Systems Using Sessile Drop and Micro-CT Imaging — **Angela Goodman, Laura Dalton, Deepak Tapriyal, Dustin Crandall**

**4:00 Paper 42c:** New Applications of Solid-State Synchronous Luminescence Spectroscopy to Study Surface/Interfacial Charge Transfer in Titanium Dioxide and Metal Titanates — **Alexander Samokhvalov**

**4:15 Paper 42d:** Ultra-Smooth, Chemically Functional Silica Surfaces for Surface Interaction Measurements and Optical/Interferometry-Based Techniques — **Howard Dobbs, Kai Kristiansen, Yair Kaufman, Jeffrey Scott, Peter Duda III, Alex Schrader, Szu-Ying Chen, Jacob Israelachvili**

**4:30 Paper 42e:** Measuring Surface Forces between Micro-Drops in Microfluidic Devices and Using Direct Force Measurement — **Emily Jamieson, Joe Berry, Raymond R. Dagastine**

**4:45 Paper 42f:** Simultaneous Microscopy and Dilatational Deformation of Complex Fluid-Fluid Interfaces — **Shalaka Kale, Andrew Cope, David Goggin, Joseph R. Samaniuk**

**5:00 Paper 42g:** Direct Measurement of Diffusiophoretic Velocity of Colloidal Particles — **P Sunthar, Rakhi Dhuriya**

**5:15 Paper 42h:** New High Temperature/Pressure Surface Forces Apparatus (TP-SFA) to Study Mineral Dissolution and Restructuring Under Sub-Surface Geological Conditions — **Kai Kristiansen, Szu-Ying Chen, Howard Dobbs, Nicholas Cadirov, Alex Schrader, Roberto C Andresen Eguiluz, Yair Kaufman, J. Boles, Jacob Israelachvili**

**5:30 Paper 42i:** Electrochemical Cell Designed for in Situ Examination of Surfactant Ionic Liquid Interface Structure — **Jeffrey Klein, Evio Panichi, Burcu Gurkan**

**5:45 Paper 42j:** Effect of Slug-Trail Mimicking Solution on Silanized-Silicon Tribology — **Appu Vinod**

**(43) Panel Discussion: Chemical Process and Product Design Careers**  
**Sunday, Oct 28, 3:30 PM**  
David L. Lawrence Convention Center, 326

Kishori T. Deshpande, Chair  
Anand N. Vennavelli, Co-Chair  
Shashank Tiwari, Co-Chair

**Sponsored by:** Product Design

**3:30 Paper 43a:** Panelist Speaker Dr. Maria Pollard — **Maria Pollard**

**3:55 Paper 43f:** Panelist for Discussion on Chemical Process and Product Design Careers — **Krystle Emanuel**

**4:20 Paper 43c:** Presentation By Dr. Mu Wang — **Mu Wang**

**4:45 Paper 43d:** Presentation By Dr. Sita Krishnan — **Sitaraman Krishnan**

**5:10 Paper 43e:** Presentation By Dr. Ken Cox — **Kenneth Cox**

**(44) Particle Technology: Educational Efforts**  
**Sunday, Oct 28, 3:30 PM**  
David L. Lawrence Convention Center, 415

Karl Jacob, Chair  
Shrikant Dhodapkar, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**(45) Polymer Thin Films, Nanoconfinement, and Interfaces**  
**Sunday, Oct 28, 3:30 PM**  
David L. Lawrence Convention Center, 309

Joseph F. Stanzione III, Chair  
Stephen M. Martin, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 45a:** Quantifying Polymer and Additive Density Distributions in Ion-Conducting and Tapered Block Polymer Thin Films — **Thomas H. Epps, III, Melody Morris, Thomas Gartner III**

**4:00 Paper 45b:** Properties of Cyclic, Linear, and Topological Blend Films of Poly(e-caprolactone) — **Giovanni M. Kelly, Amelia Bergeson, Fariyah M. Haque, Scott M. Grayson, Julie N. L. Albert**

**4:15 Paper 45c:** Understanding Artificial Touch: Designing "Softness" and Molecular Discriminability for Haptic Devices — **Charles Dhong, Rachel Miller, Ryan Arroyo, Cody Carpenter, Nicholas Root, Darren Lipomi**

**4:30 Paper 45d:** Designing Biomimetic Polymeric Interfaces: Using Photopolymerization Techniques to Simultaneously Control Surface Chemistry, Topography and Functionality — **Caroline Szczepanski, Thierry Darmanin, Frédéric Guittard, Guilhem Godeau, John M. Torkelson**

**4:45 Paper 45e:** Laser Induced Buckling for Microscale Patterning — **Kunal Mondal, Michael D. Dickey, Jan Genzer**

**5:00 Paper 45f:** Tg and Structural Recovery of Nanoconfined Polystyrene — **Madhu Pallaka, Yung P. Koh, Sindee L. Simon**

**5:15 Paper 45g:** Investigating Polymeric Thin Film Vapour Uptake and Their Properties Using the Quartz Crystal Microbalance — **Mark A. Isbell, Geoff G. Z. Zhang, Jerry Y. Y. Heng**

**5:30 Paper 45h:** Compositionally Versatile Polymer Thin Films for pH-Responsive Properties and Metal Capture — **Xuanli Deng, Nathan Spear, G. Kane Jennings**

**5:45 Paper 45i:** Adhesion Hysteresis of Polystyrene Thin Films — **George Degen, Thomas R. Cristiani, Nicholas Cadirov, Roberto C Andresen Eguiluz, Jacob Israelachvili**

**(46) Reaction Engineering for Combustion and Pyrolysis**  
**Sunday, Oct 28, 3:30 PM**  
David L. Lawrence Convention Center, 402

Bihter Padak, Chair  
C. Franklin Goldsmith, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 46a:** Changes in Characteristic Parameters of Co-Fired Biomass and Coal Particles Exposed to Oxy-Fired and High Pressure Conditions — **Lauren Kolczynski, Alexander Prlina, Schuyler McFall, Abby Hall, Eric Eddings, Terry Ring**

**3:52 Paper 46b:** Investigation of Bimetallic Mn-Fe Oxygen Carriers for Coal in Situ Gasification Chemical-Looping Combustion (iG-CLC) — **Ping Wang, Nicholas C. Means, Bret H. Howard, Dushyant Shekhawat**

**4:14 Paper 46c:** An Examination of HONO and HNO<sub>2</sub> in Low-Temperature Combustion — **Mark Fuller, C. Franklin Goldsmith**

**4:36 Paper 46d:** Pyrolytic Remediation of Oil-Contaminated Soils: Reaction Mechanisms and Treated Soil Fertility — **Julia E. Vidonish, Pedro J. J. Alvarez, Kyriacos Zygourakis**

**4:58 Paper 46e:** Effect of Temperature and Transport on the Yield and Composition of Pyrolysis-Derived Bio-Oil — **Khurshed B. Ansari, Jyotsna S. Arora, Jia Wei Chew, Paul J. Dauenhauer, Samir H. Mushrif**

**5:20 Paper 46f:** Comparison between Catalytic Fast Pyrolysis and Catalytic Fast Hydrolysis of Arundo Donax in a Fluidized Bed Reactor — **Devin Chandler, Fernando Resende**

**5:42 Paper 46g:** A Framework for Chemical Kinetics Extraction Based on Reactive Molecular Dynamics — **Srujan Rokkam, Kiran Sasikumar, Raghavan Ranganathan, Peter Cross, Richard Burnes**

**(47) Reaction Path Analysis**  
**Sunday, Oct 28, 3:30 PM**  
David L. Lawrence Convention Center, 404

Michael T. Klein, Chair  
Preetinder S. Virk, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 47a:** Magnetic Imaging to Model Olefin Product Yields from High Severity Naphtha Cracking — **Preetinder S. Virk**

**3:52 Paper 47b:** Reaction Coupling of Propane Dehydrogenation and Nitrobenzene Hydrogenation — **Peng Yu, Hsi-Wu Wong**

**4:14 Paper 47c:** Tuning Solid Catalysts to Control Regioselectivity in Cross-Aldol Condensations with Unsymmetrical Ketones — **Koushik Ponnuru, Jinesh Manayil, Hong Je Cho, Wei Fan, Karen Wilson, Friederike C. Jentoft**

**4:36 Paper 47d:** Microkinetic Analysis of Ethylene Hydrogenation on Pd-Based Catalysts: Effect of Subsurface Hydrogen on Mechanism and Rate Control — **Gamze Gumuslu-Gur, James B. Miller, Andrew J. Gellman**

**4:58 Paper 47e:** Importance of Explicit Solvent Molecule Inclusion in Predicting Electrolyte Reduction Kinetics in Lithium Ion Batteries — **Mathew J. Boyer, Gyeong S. Hwang**

**5:20 Paper 47f:** Software Tools for Developing Molecular-Level Kinetic Models of Large, Complex Chemical Systems — **Pratyush Agarwal, Juan Lucio-Vega, Michael T. Klein**

#### (48) Reactor Engineering for Biomass Feedstocks

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 317

Yukihiko Matsumura, Chair  
Quang Nguyen, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**3:30** Introductory Remarks

**3:36 Paper 48a:** Degradation of Lignocellulose and Production of Chemicals Via Sequential Hydrothermal Liquefaction — **Xiangyu Gu, Shulin Chen**

**4:00 Paper 48b:** Reaction Mechanism of Retro-aldol Condensation under Hydrothermal Condition — **Rahmat I. Mainil, Nattacha Paksung, Yukihiko Matsumura**

**4:24 Paper 48c:** Catalytic Upgrading of Algae Bio-Oil from Hydrothermal Liquefaction on Ni-Based Catalyst: The Role of Support — **Kanokthip Pongsiriyakul, Worapon Kiatkittipong, Sushil Adhikari, Kunlanan Kiatkittipong, Navadol Laosiripojana, Kajornsak Faungnawakij, Suttichai Assabumrungrat**

**4:48 Paper 48d:** Jet Biokerosene Obtained from Babassu Vegetable Oil Using Molecular Distillation — **Vanessa Oliveira, F. Murilo T. Luna, Expedito Parente Jr., Célio L. Cavalcante Jr.**

**5:12** Break

**5:36 Paper 48f:** Microbial Network Analysis Using Co-Occurrence Patterns of Methanogens and Bacteria in Full-Scale Biogas Plants — **Okkyoung Choi, Hyejeong Song, Hyunook Kim, Byoung Seung Jeon, Byoung-In Sang**

#### (49) Rechargeable / Secondary Battery Technologies for Energy Storage

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 324

Jason Morgan, Chair  
Ryan Anderson, Co-Chair

**Sponsored by:** Transport and Energy Processes

**3:30 Paper 49a:** Modeling the Effect of Mesoporous Carbon Cathodes in Li-S Batteries — **George Shebert, Yong Lak Joo**

**3:45 Paper 49b:** Theoretical and Experimental Characterizations of a Rechargeable Hybrid Cathode for Lithium-Based Batteries — **Sarwan S. Sandhu, Joseph P. Fellner, Clayton Cashion**

**4:00 Paper 49c:** Autocatalytic Reactions and Surface Diffusion Control Phase Separation in  $\text{Li}_x\text{FePO}_4$  — **Yiyang Li, Jongwoo Lim, Martin Z. Bazant, William Chueh**

**4:15 Paper 49d:** Passivated Lithium Anodes of Lithium Sulfur Batteries with Modified Electrolyte Containing Transition Metal Acetate — **Wenduo Zeng, Mark Cheng, Simon Ng**

**4:30 Paper 49e:** Optimal Thermal Management of a High-Temperature Sodium Sulphur Battery — **Sai Pushpitha Vudata, Debangsu Bhattacharyya, Richard Turton**

**4:45 Paper 49f:** Stochastic Statistical Models of Vehicle-to-Grid Economics for Predicting Impact of Policy and Renewables Portfolio — **Heta Gandhi, Andrew White**

**5:00 Paper 49g:** Tailoring Battery Electrode Resistance to Combat Dendrite Formation — **Neda Seyedhassantehrani, James W. Palko**

**5:15 Paper 49h:** Electrochemical and Thermal Modeling of Capacity Fade in Lithium Ion Batteries for Prognosis — a Reaction Kinetic Approach — **Parth Shah Devalkumar, Sathish Swaminathan, Resmi Suresh, Raghunathan Rengaswamy**

#### (50) Self-Assembly in Solution

**Sunday, Oct 28, 3:30 PM**

Omni William Penn Hotel, Conference Center A

Claribel Acevedo, Chair  
Kenneth Mineart, Co-Chair  
Paschalis Alexandridis, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 50a:** Using Oxidation State-Dependent Self-Assembly of Ferrocenyl Surfactants to Enhance Efficiency of Light Energy Harvesting — **Nicholas L. Abbott, Timothy Smith**

**3:45 Paper 50b:** Self-Assembly of Biomimetic Nanoparticles — **Nicholas Kotov**

**4:00 Paper 50c:** Self-Assembly of Fluorinated Surfactants — **Samhitha Kancharla, Dmitry Bedrov, Paschalis Alexandridis**

**4:15 Paper 50d:** Tuning Self-Assembled Block Copolymer Micelles Via Co-Solvent Addition — **Tyler J. Cooksey, Xiuli Li, Avantika Singh, Kim Mai Le, Elizabeth G. Kelley, Sameer Vajjala Kesava, Enrique D. Gomez, Bryce E. Kidd, Louis Madsen, Megan L. Robertson**

**4:30 Paper 50e:** Exploiting Amphiphile Interactions with Polyelectrolyte/Multivalent Ion Coacervates in Long-Term Sustained Release — **Udaka K. de Silva, Jennifer L. Brown, Yakov Lapitsky**

**4:45 Paper 50f:** Solubilization of Limonene into Aqueous Solutions of Dialkyl Phosphatidylcholine Micelles — **Andrew P. Karman, Stephanie R. Dungan, Susan E. Ebeler, Nitin Nitin**

**5:00 Paper 50g:** Modeling a Mixture of Multi-Bonding Site Solute and Patchy Colloidal Solvent in Confined Systems — **Yuchong Zhang, Yiwei Zhu, Dilip Asthagiri, Walter G. Chapman**

**5:15 Paper 50h:** Phase and Rheological Behavior of Aqueous Mixtures of an Isopropoxylated Surfactant — **Jaeyub Chung, Yung-Jih Yang, Huiling Tang, Marika Santagata, Bryan W. Boudouris, Elias I. Franses**

**5:30 Paper 50i:** Composition-Driven Structural Transitions from Vesicles to Bicelles to Micelles Using Phospholipid and Nonionic Surfactant Mixtures — **Igor Kevin Mkam Tsengam, Marzhana Omarova, Srinivasa R. Raghavan, Geoff Bothun, Alon McCormick, Vijay T. John**

**5:45 Paper 50j:** Solvatochromic Property in Lipid Bilayer Interphases Analyzed Based on Time Resolved Emission Spectrum of Laurdan — **Nozomi Watanabe, Keishi Suga, Thomas Nyholm, J. Peter Slotte, Hiroshi Umakoshi**

#### (51) Software Tools and Implementations for Process Systems Engineering

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 410

Benoit Chachuat, Chair  
Bethany Nicholson, Co-Chair

**Sponsored by:** Computing Systems and Technology Division

**3:30 Paper 51a:** Pynumero: Python Numerical Optimization — **Jose S. Rodriguez, Bethany Nicholson, Carl D. Laird, John D. Sirola**

**3:49 Paper 51b:** Graph-Based Modeling Abstractions and Computational Tools for Complex Systems — **Jordan Jalving, Victor M. Zavala**

**4:08 Paper 51c:** Plasmalgorithms, a Collection of Decomposition Algorithms for Graph-Based Problem Representations — **Braulio Brunaud, M. Paz Ochoa, Alisandra Welch, Ignacio E. Grossmann**

**4:27 Paper 51d:** Component Based Development of Application Specific Computer-Aided Tools — **Anjan Kumar Tula, Mario Richard Eden, Rafiqul Gani, Xi Chen**

**4:46 Paper 51e:** SPICE: A Computer-Aided Platform for Simultaneous Process Synthesis and Intensification — **Jianping Li, Salih E. Demirel, M. M. Faruque Hasan**

**5:05 Paper 51f:** Data Driven Modeling in Alamo: Feature Selection and Non-Parametric Modeling Applications — **Zachary Wilson, Nick Sahinidis**

**5:24 Paper 51g:** Recent Advances in the EaGO Platform: Global and Robust Optimization in Julia — **Matthew Wilhelm, Matthew D. Stuber**

**5:43 Paper 51h:** A Sensitivity-Based Nonlinear Model Predictive Control and State-Estimation Framework in Python — **David Thierry, Bethany Nicholson, Lorenz T. Biegler**

## (52) Supply Chain Design and Logistics

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 409

Xiang Li, Chair  
Ajit Gopalakrishnan, Co-Chair

**Sponsored by:** Computers in Operations and Information Processing

**3:30 Paper 52a:** Multi-Period Design and Planning of Centralized and Distributed Manufacturing Networks — **Cristiana L. Lara**, Christian Wende, Ignacio E. Grossmann

**3:49 Paper 52b:** A Stochastic Game Theoretic Framework for Optimization of Decentralized Supply Chains Under Uncertainty — **Jiyao Gao**, Fengqi You

**4:08 Paper 52c:** A Column Generation Approach to Multiscale Capacity Planning for Continuous Power-Intensive Processes — **Angela Flores-Quiroz**, Jose M. Pinto, Qi Zhang

**4:27 Paper 52d:** Solving Robust Vehicle Routing Via a Branch-Price-and-Cut Approach — **Akang Wang**, Chrysanthos E. Gounaris

**4:46 Paper 52e:** Autologous Cancer Therapies: How Can We Handle the Complexity of the Supply Chain? — **Maria M. Papathanasiou**, Nilay Shah

**5:05 Paper 52f:** Surrogate-Based Derivative-Free Optimization of a Multi-Enterprise Supply Chain Simulation — **Atharv Bhosekar**, Marianthi Ierapetritou

**5:24 Paper 52g:** Strategic Time Window Assignment in Vehicle Routing Operations — **Anirudh Subramanyam**, Akang Wang, Chrysanthos E. Gounaris

**5:43 Paper 52h:** Time Window Based Berth and Yard Allocation Planning of Container Vessels — **Jialin Xu**, Honglin Qu, Qiang Xu

## (53) Thermodynamics of Polymers

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 327

Eric W. Cochran, Chair  
Kathleen McEnnis, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 53a:** Collapse and Swelling of Polymer Chains in Mixed Solvents Near the Critical Point — **Xiong Zheng**, Mikhail A. Anisimov, Jan V. Sengers, Maogang He

**3:45 Paper 53b:** Modeling of Solution Thermodynamics: A Method for Tuning the Properties of Blend Polymeric Membranes — **Krishnasri Kurada**

**4:00 Paper 53c:** Liquids That Freeze When Mixed: Co-Crystallization and Liquid-Liquid Equilibrium in Polyoxacyclobutane-Water Mixtures — **Joyita Banerjee**, Peter Koronaos, Robert M. Enick, John A. Keith, Eric J. Beckman, Sachin Velankar

**4:15 Paper 53d:** Self-Assembly of Ordered Networks in Block Copolymer Systems Using Coarse-Grained Simulations — **Natalie Buchanan**, Poornima Padmanabhan

**4:30 Paper 53e:** Phase Behavior of AB/CD Diblock Copolymer Blends Via Coarse-Grained Simulations — **Iman Ahmadian**, Andrew Peters

**4:45 Paper 53f:** Extreme Architectural Asymmetry with Miktoarm Star Polymers: Tough Thermoplastic Elastomers and Frank-Kasper Phases — **Joshua Lequieu**, Kris Delaney, Glenn H. Fredrickson

**5:00 Paper 53g:** Phase Behavior of Pyrene and Vinyl Polymers with Aromatic Side Groups — **Gagan N. Kangovi**, Sangwoo Lee

**5:15 Paper 53i:** Bonded Potentials of Coarse-Grained Polymer Models — **Qiang (David) Wang**

**5:30 Paper 53j:** Mechanistic Understanding of the Thermal and Barrier Properties of PET and PEF Via Computation — **Brandon C. Knott**, Graham Schmidt, Phillip Hudson, Gregg T. Beckham, H. Lee Woodcock, Michael F. Crowley, Benjamin Pollard

## (54) Workshop: Best Practices in Research Mentoring

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 413

Adrienne Minerick, Chair  
Daniel Lepek, Co-Chair

**Sponsored by:** Graduate Education

## (55) Workshop: Effective Teaching for New or Prospective Faculty

**Sunday, Oct 28, 3:30 PM**

David L. Lawrence Convention Center, 411

David L. Silverstein, Chair  
Lisa G. Bullard, Co-Chair  
Donald P. Visco Jr., Co-Chair

**Sponsored by:** Undergraduate Education

**3:30** Welcoming Remarks

**3:35** Workshop

## (56) 3D Printing II

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 333

Lin Li, Chair  
Nima Yazdanpanah, Co-Chair

**Sponsored by:** 3D Printing

**8:00 Paper 56a:** 3D Printed Complex Dosage Forms Embedded with Engineered BCS Class II Drug Particles — **Guluzar Gorkem Buyukgoz**, Marian Abdelmalak, Rahul Kapoor, Jeremiah Castro, Shen Ji, Scott Quirie, Murat Guvendiren, Rajesh Davé

**8:20 Paper 56b:** 3D Printing for Rapid Prototyping of Innovative Process Equipment for Pharmaceutical Crystallization — **Kiran Mathew Thomas**, Dong ik Shin, Richard Lakerveld

**8:40 Paper 56c:** Direct Write of UV Curable Polymer Bonded Magnets — **Alan Shen**, Anson Ma, Sameh Dardona, Callum Bailey

**9:00 Paper 56d:** Before You Click "Print": Regulatory Considerations for 3D Printed Oral Drug Products — **Ahmed Zidan**, Alaadin Alayoubi, James Coburn, Bahaa Ghamraoui, Celia N. Cruz, Muhammad Ashraf

**9:20 Paper 56e:** Two-Color Photo-Inhibited Systems for Rapid Additive Manufacturing — **Martin de Beer**, Harry van der Laan, Riley Whelan, Timothy F. Scott, Mark A. Burns

**9:40 Paper 56f:** Glass-Forming Polymer Networks for Shape-Memory Contact Printing — **Mitchell Anthamatten**, Xinquan Chen, Dezhi Liu

## (57) Advances in Functional Food Production

**Monday, Oct 29, 8:00 AM**

Westin Convention Center, Westmoreland East

Hesham EL Enshasy, Chair  
Liqing Zhao, Co-Chair

**Sponsored by:** Food

**8:00 Paper 57a:** Infusion of Walnut Husk into Polyethylene — **Jonathan E. Wenzel**, Scott Constine, Kirsten Cussans, Elijah Ward, Lihua Wang, Cheryl Samaniego, Michelle Ammerman

**8:18 Paper 57b:** Extraction of Bromelain from Pineapple (Ananas Comosus) Using Membrane Filtration — **Ani Idris**

**8:36 Paper 57c:** Implementation of a Mixed Integer Linear Programming Approach to Establish *De Novo* Synthesis Routes of Antioxidants Derived from the Fermentation of *Theobroma Cacao* Seeds — **Lina J. Suarez Medina**, **Andrés Fernando González Barrios**, Jorge M. Gómez, Oscar A. Alvarez, José González-Valdez, Marco Rito-Palomares, Alejandro Caro Quintero, María C. García Muñoz, Hector H. Olarte Noreña, Silvia Restrepo, Martha J. Vives Florez, Alejandro Reyes Muñoz

**8:54 Paper 57d:** Encapsulation of Lactic Acid Bacteria By Multiple Emulsion System — **Chia C. Hsu**, Nai Y. Wang, Yu C. Cheng, Jinn T. Lai

**9:12 Paper 57e:** Optimization of Process Parameters for Protease Production From Thermophilic Bacterial Strain Isolated from Hot Water Springs in Oman — **Hamed Saed Khaleifin Al Maqhusi**, Sheikh Saif Humoud Nasser Al Harthi, Marwa Al Farsi, **Awnish Pareek**, Taqi Ahmed Khan, Hesham EL Enshasy

**9:30 Paper 57f:** Production of Heavy Oil Liamocin By *Aureobasidium Pullulans* — **Zhen Qin**, Xin Liu, Shang-Tian Yang

**9:48 Paper 57g:** (Keynote) Efficient Biosynthesis of Omega-3 PUFA: From Lab to Factory — **He Huang**

## (58) Analysis and Design of Carbon Dioxide Capture Technologies for Power Generation

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 321

David Hopkinson, Chair  
Zachary P. Smith, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**8:00 Paper 58a:** U.S. DOE National Energy Technology Laboratory: Carbon Capture R&D Program's New Direction for Operational Versatility — **José D. Figueroa**, Lynn Brickett, Kanwal Mahajan

**8:18 Paper 58b:** Highlights of Collaboration between the U.S. DOE Carbon Capture Simulation for Industry Impact Program and the Discovery of Carbon Capture Substances and Systems Initiative — **Michael S. Matuszewski**, Benjamin P. Omell, David C. Miller, Debangsu Bhattacharyya, Rebecca Siegelman, Jeffrey R. Long, Charles J. Freeman, Zhijie Xu, Joshua Stolaroff



**8:36 Paper 58c:** Process Modeling and Experimental Studies of a Diamine-Appended Metal–Organic Framework for CO<sub>2</sub> Capture  
— **Ryan Hughes**, Goutham Kotamreddy, Debansu Bhattacharyya, Michael S. Matuszewski, Rebecca Siegelman, Jeffrey R. Long

**8:54 Paper 58d:** Analysis of Different Solvent Performance in UKy-CAER's 0.7 MWe CO<sub>2</sub> Capture Pilot Plant  
— **Reynolds A. Frimpong**, Heather Nikolic, Jonathan V. Pelgen, Kunlei Liu

**9:12 Paper 58e:** *In-Situ* Gasification Chemical Looping Combustion vs. Chemical Looping with Oxygen Uncoupling: Exergy Comparison for Power Generation with CO<sub>2</sub> Capture  
— **Yitao Zhang**, Andrew Tong

**9:30 Paper 58f:** The Development of Machine Learning, Group Contribution and Molecular Modeling Approach to Screen Physical Solvents for Gas Separation  
— **Wei Shi**, Megan Macala, Robert L. Thompson, Surya Tiwari, Kevin P. Resnik, Nicholas Siefert, David Hopkinson

**9:48 Paper 58g:** Towards the Development of a Solvent Screening Tool for CO<sub>2</sub> Capture Using Molecular Thermodynamics  
— **Luis M.C. Pereira**, Félix Llovel, Ismail I. Alkhatib, Lourdes F. Vega

**10:06 Paper 58h:** Systematic Design of Phase-Change Solvents for Post-Combustion CO<sub>2</sub> Capture Based on Advanced Thermodynamics and Holistic Sustainability Assessment  
— **Athanasios I. Papadopoulos**, Gulnara Shavaliyeva, Felipe Perdomo-Hurtado, Panos Seferlis, Stavros Papadokostantakis, Claire S. Adjiman, Amparo Galindo, George Jackson

**(59) Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering I (Invited Talks)**  
**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 327

Amy M. Peterson, Chair  
Julie N. L. Albert, Co-Chair

**Sponsored by:** Polymers

**8:00 Paper 59a:** Advances in Intelligent Hydrogels for Biomedical Applications  
— **Nicholas A. Peppas**, Julia Vela Ramirez, Matthew Miller

**8:35 Paper 59b:** Bioinspired Materials for Musculoskeletal Tissue Engineering  
— **Julianne L. Holloway**

**9:10 Paper 59c:** Colloidal Surface Stabilization Ability of Zwitterionic Copolymers  
— **Margarita Herrera-Alonso**

**9:45 Paper 59d:** Molecular Engineering of Polymers for Electrochemical Applications in Water and Energy  
— **Christopher G. Arges**, Yupo J. Lin, Varada Menon Palakkal, Le Zhang

**(60) Area Plenary: Interfacial Phenomena (Invited Talks)**

**Monday, Oct 29, 8:00 AM**  
Omni William Penn Hotel, Conference Center A

Raymond Tu, Chair  
Marina Tsianou, Co-Chair

**Sponsored by:** Interfacial Phenomena

**8:00 Paper 60a:** Contact and Adhesion at Soft and Structured Interfaces  
— **Joelle Frechette**

**8:50 Paper 60b:** Effect of the Surfactant Molecular Structure on the Stabilization of Colloidal Suspensions Against Agglomeration and Sedimentation  
— **Elias I. Franses**

**9:40 Paper 60c:** Complex Polymer Architectural Designs for Interfacial Engineering  
— **Robert D. Tilton**

**(61) Area 8D (Inorganic Materials) Graduate Student Award Session**

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 329

Kumar Varoon Agrawal, Chair  
Xueyi Zhang, Co-Chair

**Sponsored by:** Inorganic Materials

**8:00 Paper 61a:** Electrical Energy Generation Via Reversible Chemical Doping on Transition Metal Dichalcogenide Thin Films – a Wearable H<sub>2</sub>O Voltage Generator  
— **Albert Tianxiang Liu**, Yuichiro Kunai, Anton Cottrill, Michael Strano

**8:30 Paper 61b:** Dual Role of Surfactants in Zeolite Synthesis and Catalyst Optimization  
— **Aseem Chawla**, Rui Li, Rishabh Jain, R. John Clark, James Sutjianto, Jeremy Palmer, Javier García-Martínez, Jeffrey D. Rimer

**9:00 Paper 61c:** *Broadening the Scope of Fluoride-Free Siliceous Zeolite Synthesis*  
— **Vivek Vattipalli**, Abdul Paracha, Weiguo Hu, Huiyong Chen, Wei Fan

**9:30 Paper 61d:** Ultrafast Synthesis of High-Silica Erionite Zeolite As a Catalyst for NH<sub>3</sub>-SCR  
— **Jie Zhu**, Zhendong Liu, Kenta Iyoki, Chokkalingam Anand, Kaname Yoshida, Yukichi Sasaki, Sohei Sukenaga, Mariko Ando, Hiroyuki Shibata, Takeshi Ohnishi, Masaru Ogura, Tatsuya Okubo, Toru Wakihara

**(62) Big Data and Sustainability**

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 315

William M. Barrett, Chair  
Nastassja Lewinski, Co-Chair

**Sponsored by:** General

**8:00 Paper 62a:** A Model-Based Sustainability Study of Energy Consumption, Environmental Pollution, and Economic Growth in China  
— **Jianming Geng**, Nengxin Wang, Kaiyuan Chen, Sihan Ling, Zuyi (Jacky) Huang

**8:26 Paper 62b:** Linking Molecular Structure to Functional Group and Chemical Literature Using a Chemical Reaction Database  
— **William M. Barrett**, Sudhakar Takkellapati, Kidus Tadele, Leora Vegosen, Michael A. Gonzalez

**8:52 Paper 62c:** Sustainability Identification for Infinite-Dimensional Systems  
— **Masih Jorat**, Vasilios Manousiouthakis

**9:18 Paper 62d:** Environmental Genome: New Database for Public Health and Chemical/Materials Manufacturing  
— **Michael Overcash**, Evan M.H. Griffing, Eric Vozzola, Matthew Realf, Concepcion Jimenez-Gonzalez

**9:44 Paper 62e:** Toward a Leading Indicator of Catastrophic Shifts in Complex Systems: Assessing Changing Conditions in Nation States  
— **Leisha Vance**, Tarsha Eason, Heriberto Cabezas, Michael Gorman

**(63) Biobased Fuels and Chemicals: Biosynthetic Pathway Engineering & Enzymatic Conversion**

**Monday, Oct 29, 8:00 AM**  
Westin Convention Center, Westmoreland West-Central

Han Li, Chair  
Joshua K. Michener, Co-Chair

**Sponsored by:** Bioengineering

**8:00 Paper 63a:** Computational Protein Design Enables Efficient Regeneration of a Biomimetic Cofactor to Support Diverse Redox Chemistries  
— **William Black**, Wai Shun Mak, Linyue Zhang, Sarah Maxel, Bonnie Fong, Justin Siegel, Han Li

**8:18 Paper 63b:** Cell-Free Metabolic Engineering for Heterologous Pathway Optimization in *Pseudomonas Putida* KT2440  
— **Joseph Rollin**, Christopher Johnson, Peter St. John, Paul E. Abraham, Robert Hettich, Gregg T. Beckham

**8:36 Paper 63c:** Application of Enzyme Promiscuity to Establish Non-Natural Biosynthetic Pathways for the Production of Phenolic Compounds  
— **Qipeng Yuan**

**8:54 Paper 63d:** Polyketide Synthases As a Platform for Biofuel Production  
— **Amin Zargar**, Constance Bailey, Ravi Lal, Miranda Werts, Jessica Wang, Andrew Wong, Satoshi Yuzawa, Leonard Katz, Jay Keasling

**9:12 Paper 63e:** High-Throughput, Mass Spectrometry-Based Screening of Microbial Libraries to Produce Designer Free Fatty Acids with Custom Compositions  
— **Tong Si**, Jonathan V. Sweedler, Huimin Zhao

**9:30 Paper 63f:** Quantitative Whole-Cell Biocatalyst Characterization: Elucidating Structure-Performance Relationships in Cell-Surface Displayed Multi-Enzyme Assemblies  
— **Mason Smith**, Hui Gao, Fei Wen

**9:48 Paper 63g:** Olfactory Receptor-Based Sensors to Accelerate the Engineering of Chemical-Producing Microbes  
— **Pamela Peralta-Yahya**

**(64) Biomaterials**

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 311

Whitney L. Stoppel, Co-Chair  
Kelly A. Burke, Co-Chair  
Kaitlin Bratlie, Co-Chair  
Christopher A. Alabi, Co-Chair

**Sponsored by:** Biomaterials

**8:00 Paper 64a:** Improving Cardiac Function after Myocardial Infarction Via Local Delivery of Mydglf Using an Injectable Polyester-Based Hydrogel  
— **Yung-Hao Tsou**, Xiaoyang Xu

**8:18 Paper 64b:** Adhesive and Electroconductive Cardiac Patches for Cardiac Tissue Regeneration Following Myocardial Infarction  
— **Brian Walker**, Chu Yu, Roberto Portillo Lara, Ehsan Shirzaei Sani, Nasim Annabi

**8:36 Paper 64c:** Mid-Infrared Laser-Activated Tissue Sealing Using Biomaterials  
— **Inam Ridha**, Ali Basiri, Deepanjan Ghosh, Jung Keun Lee, Jacquelyn Kilbourne, Yu Yao, Kaushal Rege

**8:54 Paper 64d:** Microscopic and *in Vitro* Testing of a Chitosan-Based Bone Adhesive  
— **Jose German Vargas**, Laura Andrea Gomez, Julian Andres Serna, Juan Carlos Cruz Jimenez, Carolina Muñoz-Camargo, Juan Carlos Briceño Triana

**9:12 Paper 64e:** *In Vitro* Reconstitution of Natural Mucins Captures pH and Ion-Dependent Collective Dynamic Mucus Barrier Complexity — *Abhinav Sharma, Neil S. Forbes, Jungwoo Lee*

**9:30 Paper 64f:** Structure-Function Analysis of Phenylpiperazine Derivatives As Intestinal Permeation Enhancers — *Katherine Fein, Nicholas G. Lamson, Kathryn A. Whitehead*

**9:48 Paper 64g:** Incorporating Electrospun Fiber Topography in a 3D PEG Hydrogel Promotes Oligodendrocyte Maturation — *Lauren Russell, Ethan Purnell, Kyle Lampe*

**10:06 Paper 64h:** Engineered Biomaterials for Thermal Stabilization of Biomolecules — *Balaji V. Sridhar, John R. Janczy, Bruno Marco Dufort, Mark W. Tibbitt*

**(65) Biomaterials and Life Science Engineering: Faculty Candidates**  
**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 328

Shannon L. Servoss, Co-Chair  
Helen Zha, Co-Chair

Julianne L. Holloway, Co-Chair

**Sponsored by:** Biomaterials

**8:00 Paper 65a:** Triggerable Tissue Depth of Externally-Triggerable Drug Delivery Systems for on-Demand Nerve Block — *Alina Rwei*

**8:18 Paper 65b:** Approaches for Creating Smart Insulin Delivery Systems — *Lisa R. Volpatti, Morgan Matraaga, Abel B. Cortinas, Robert Langer, Daniel G. Anderson*

**8:36 Paper 65c:** Biomolecular Engineering of Acousto-Magnetic Protein Nanostructures for Non-Invasive Imaging of Cellular Function — *George J. Lu, Arash Farhadi, Jerzy O. Szablowski, Audrey Lee-Gosselin, Samuel R. Barnes, Anupama Lakshmanan, Raymond W. Bourdeau, Mikhail G. Shapiro*

**8:54 Paper 65d:** A New Antifouling Strategy with Active Surface Topography — *Huan Gu, Sang Lee, Dacheng Ren*

**9:12 Paper 65e:** Developing Platform Biomaterials: From Messenger RNA Delivery to User-Friendly Synthetic Hydrogels — *Owen S. Fenton, Robert Langer*

**9:30 Paper 65f:** Enzymatically Powered Surface-Associated Self-Motile Protocells — *Woo-Sik Jang, Hyun Ji Kim, Chen Gao, Daeyeon Lee, Daniel A. Hammer*

**9:48 Paper 65g:** Rational Fabrication of Polymer-Graphene Based Scaffolds/Devices Using 3D Bioprinting and Microfluidics to Control Stem Cell Differentiation and Fate Commitment — *Metin Uz*

**10:06 Paper 65h:** Using Biological Heterogeneity to Understand Disease: From Single Cells to Personalized Medicine — *Daniel Cook*

**(66) Biotechnology & Materials U.G. Research Session (Invited Talks)**

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 302

Shelby Brooks, Chair  
Ashiqur Rahman, Co-Chair

**Sponsored by:** Young Professionals Committee (YPC)

**8:00 Paper 66a:** Design of Experiments Study to Formulate Dry Powder Aerosols for Bacterial Biofilm Eradication — *Ojas Pradhan*

**8:25 Paper 66b:** Biohybrid Microswimmers with Biocompatible Polymetric Multilayers as Drug Delivery System — *Katelyn M Bevilacqua, Guraarashjot S Multani, Byung-Wook Park*

**8:50 Paper 66c:** Examining chitosan-titanium bonding with various addition in heated simulated body fluid — *Patrick McWhorter*

**9:15 Paper 66d:** Fabrication of Transition Metal Chalcogenide Cu<sub>2</sub>Se Semiconducting Thin Films and Thermoelectric Property Characterization — *Nan (Louise) Chen*

**9:40 Paper 66e:** A New Way to Model the Brain: The Flow Limiting Operator — *Jeffrey Horbatiuk*

**10:05 Paper 66f:** Engineering Topography to Direct Oligodendrocyte Precursor Cell Fate — *Ethan Purnell*

**(67) Carbon Dioxide Capture Technologies and Their Use I**

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 319

Sunil Hangal, Chair  
Gonzalo Guillén-Gosálbez, Co-Chair

**Sponsored by:** Climate Change

**8:00 Paper 67a:** On the Role of Fe<sup>2+</sup> and O<sub>2</sub> in Oxidative Degradation of Aqueous Monoethanolamine (MEA) — *Haley Stowe, Gyeong S. Hwang*

**8:19 Paper 67b:** Amine-Functionalized Hierarchical Zeolites for Carbon Dioxide Capture — *Maryam Khaleel, Anna Tuneu-Pujolras, Issam Ismail, Georgios N. Karanikolos, Lourdes F. Vega, Fèlix Lovell*

**8:38 Paper 67c:** Improving Full-Scale Models of New Carbon Capture Technologies with Uncertainty Quantification — *Christopher Russell, K. Sham Bhat, Joel D. Kress, Larry L. Baxter, Charles J. Freeman, Joshua C. Morgan*

**8:57 Paper 67d:** Evaluating Methane Pyrolysis As a Component for CO<sub>2</sub> Emission Negative Renewable Energy — *Fensterle Joachim, Franziska Meiners, Frank Platte*

**9:16 Paper 67e:** Development of an Integrated Mass Transfer and Kinetic Model from Multi-Scale Data for CO<sub>2</sub> Capture Using Concentrated Piperazine — *Koteswara Rao Putta, Michael S. Matuszewski, David C. Miller, Benjamin P. Omell*

**9:35 Paper 67f:** Morphology of Sodium Carbonate and Its CO<sub>2</sub> Adsorption Performance: A First-Principles Investigation — *Tianyi Cai, J. Karl Johnson, Xiaoping Chen*

**9:54 Paper 67g:** Development of Nano-TiO<sub>2</sub> Promoted CaO Adsorbent for Enhanced CO<sub>2</sub> Capture at High Temperatures: Role of Crystal Level Properties — *Sanat Chandra Maiti, Chinmay Ghoroi*

**(68) Cell Culture Engineering & Process Design**

**Monday, Oct 29, 8:00 AM**

Westin Convention Center, Fayette

Aravindan Rajendran, Chair  
Tong Si, Co-Chair

**Sponsored by:** Bioengineering

**8:00 Paper 68a:** Enhanced Oxygen Transfer and Cell Growth in a Scaled-up Multiphase Continuous Bioreactor with Internal Spiroid — *Shu Fang, Paul W. Todd, Thomas R. Hanley*

**8:18 Paper 68b:** Gas Transfer Based Methodology to Scale Single Use Bioreactor Processes — *Xin Xin, Mao-Shih Liang*

**8:36 Paper 68c:** Optimization of Microalgal Oxygen Evolution within Planar Cultivation Systems — *Sina Kaabipour, Julia Lin, Clayton S Jeffries*

**8:54 Paper 68d:** A Novel Kinetic Model-Based Metabolic Flux Analysis for Antibody Producing Cell Lines — *Denizhan Yilmaz, Satish J. Parulekar, Ali Cinar*

**9:12 Paper 68e:** Metabolic Engineering of CHO Cells for Increased Mab Production — *Sarah A. Sacco, Allison G. McAtee Pereira, Kevin Smith, Michel Betenbaugh, Jamey D. Young*

**9:30 Paper 68f:** Long-Term Live Cell Imaging of Endogenous Loci by CRISPR/Cas9-mediated Knock-in of an Optimized TetO Repeat — *Ipek Tasan, Gabriela Sustackova, Liguozhang, Jiah Kim, Mayandi Sivaguru, Mohammad Hamedirad, Yuchuan Wang, Justin Genova, Jian Ma, Andrew Belmont, Huimin Zhao*

**9:48 Paper 68g:** Engineering Protein Assemblies for Energy and Health — *Fei Wen*

**(69) Cells, Organs, and Labs on a Chip I: Modeling Cell Interactions**  
**Monday, Oct 29, 8:00 AM**

Westin Convention Center, Cambria

Nitin Agrawal, Chair  
Roman Voronov, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**8:00 Paper 69a:** Engineering a Physiologically Relevant Model of the Cardiac Autonomic Nervous System — *Jonathan Soucy, Tess Torregrosa, Sanjin Husic, Nasim Annabi, Abigail Koppes, Ryan Koppes*

**8:18 Paper 69b:** Stem Cell-Based Microfluidic Model of the Blood-Brain Barrier — *Pedram Motallebnejad, Andrew Thomas, Sarah L. Swisher, Samira M. Azarin*

**8:36 Paper 69c:** Investigation of Drug Efficacy Under *in Vitro* Hypoxic Gradients in Glioblastoma Multiforme — *Md. Daud H Khan, Nitin Agrawal*

**8:54 Paper 69d:** Engineering *In Vitro* Vascularization on a Chip — *Mi Zhang, Yajie Xu, Roshini Balan, Reed Momjian, Harihara Baskaran*

**9:12 Paper 69e:** Microfluidic Co-Culture of Triple Negative Breast Cancer Cells and Adipose Stem Cells — *Sharif M. Rahman, Katie A. Render, Joshua M. Campbell, Jeffery Anderson, C. Ethan Byrne, Elizabeth Martin, Adam Melvin*

**9:30 Paper 69f:** Articular Joint on a Chip: An *in-Vitro* Co-Culture System of Cartilage and Joint Capsule Synovium to Simulate Post-Traumatic Osteoarthritis — *Yamini Krishnan, Christina P. Rossitto, Han-Hwa K. Hung, Paula T. Hammond, Alan Grodzinsky*

**9:48 Paper 69g:** Invited Speaker: Engineering Tissues for Disease and Drug Studies — *David L. Kaplan*



## (70) Cellulose-Based Materials I

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 325

Yulin Deng, Chair

**Sponsored by:** Forest and Plant Bioproducts Division

**8:00 Paper 70a:** Reducing Energy Consumption in Thermomechanical Pulp Production Using Chlorine Dioxide — **Jayg Dimayacyac**, *Rodger Beatson, ZhaoYang Yuan*

**8:25 Paper 548h:** Understandings of Thermal Transformation of Cellulose Surface and Crystalline Core By *in-Situ* Nonlinear Vibrational Spectroscopy — **Zhangyang Xu**, *Libing Zhang, Hongfei Wang, Zheming Zhang, Bin Yang*

**8:50 Paper 191s:** Fabrication and Characterization of Novel Cellulose Acetate Hollow Fiber Nanoporous Membranes Prepared Via Thermally Induced Phase Separation — **Bo Pang**, *Xiaolin Wang, Junyi Mao*

**9:15 Paper 70d:** A Method to Prepare Smooth and Uniform Lignocellulosic Nanopapers — **Zhihua Jiang**

**9:40 Paper 70e:** Hairy Cellulose Nanocrystals-Colloidal Starch Nanocomposite Coatings with Nanoengineered Viscosity Improve the Mechanical Properties of Papers: One Stone, Two Birds — **Amir Sheikh**, *Theo G. M. van de Ven*

## (71) Characterization, Modeling and Control/Optimization of Micro- and Nano-Structured Particulate Systems

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 413

M. Silvina Tomassone, Chair  
Heather N. Emady, Co-Chair  
Priscilla Hill, Co-Chair

**Sponsored by:** Particle Production and Characterization

**8:00 Paper 71a:** High Resolution Nanoparticle Sizing with Maximum a Posteriori Nanoparticle Tracking Analysis (MANTA) — **Kevin Silmore**, *Xun Gong, Michael Strano, James Swan*

**8:18 Paper 71b:** Core-Shell Graphene/Silicon Nanoparticles for Use As Lithium-Ion Battery Anodes — **M. Silvina Tomassone**, *Kurt B. Smith*

**8:36 Paper 71c:** Multiparameter Paramagnetic Particle Characterization By Dark-Field Imaging — **Abhinav Sannidhi**, *Paul W. Todd, Thomas R. Hanley*

**8:54 Paper 71d:** Numerical Study of the Evolution of Particle Size and Morphology in an Industrial Titanium Dioxide Reactor — **Astrid Boje**, *Markus Kraft*

**9:12 Paper 71e:** Multiscale Modelling and Simulation of Particle Formation through Mono-Disperse Droplet Spray Drying — **Jie Xiao**

**9:30 Paper 71f:** Atomic Structure and Stress Release Mechanism of Core-Shell Au-Pd Nanocubes — **Michael Nathanson**, *Krishan Kanhaiya, Hendrik Heinz*

**9:48 Paper 71g:** Development and Application of a Computer Simulation Package for Wet Bead Milling of Nanoscale Pharmaceutical Particles Using Population Balance and Fundamental Principles — **Husheng Yang**

**10:06 Paper 71h:** Quantitative Study of Conduction and Convection Heat Transfer Mechanisms in a Rotary Drum — **Manogna Adepu**, *Heather N. Emady*

## (72) Characterization of Composites

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 330

Zhen Liu, Chair  
Lalitha Ganapatibhotla, Co-Chair  
Liwen Mu, Co-Chair  
Zhaofeng Wang, Co-Chair

**Sponsored by:** Composites

**8:00 Paper 72a:** Isolating the Effect of Polymer-Filler Interaction on Polymer Composite Property Enhancement: The Example of Polypropylene/Halloysite Composites — **Tong Wei**, *Kailong Jin, John M. Torkelson*

**8:18 Paper 72b:** Morphological Characteristics and Mechanical Properties of Thermoplastic Composites Using Surface Modified Cellulose Nanofibril (CNF) Fillers — **Carlos Landaverde-Alvarado**, *Rebecca Martin, Benjamin Beck, Stephen M. Martin*

**8:36 Paper 72c:** Alternative Methodology for Characterizing Tool-Ply Friction of Unidirectional Carbon Fiber - Epoxy Prepregs at Various Processing Conditions — **Michael J. Bortner**, *Kathleen Chan, Davide De Focatiis, David Dillard*

**8:54 Paper 72d:** Thermomechanical Behavior of Polymer Films at Cryogenic Temperatures — **Bo Bonning**, *Jordan Blackburn, Holly A. Stretz, Chris Wilson*

**9:12 Paper 72e:** Nanoscale Structure-Property Relationships of Polyacrylonitrile/CNT Composites As a Function of Polymer Crystallinity and CNT Diameter — **Jacob Gissinger**, *Chandrani Pramanik, Bradley Newcomb, Satish Kumar, Hendrik Heinz*

**9:30 Paper 72f:** The Dynamic Mechanical Performance of Glass Fiber Reinforced Thermoplastic Composites — **Chunyin Shen**, *Haiping Wan, Junyan Wang, Yanqing Ding, Bin Lee, Gance Dai*

## (73) Combustion Kinetics and Emissions

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 402

Bihter Padak, Chair  
Erdem Sasmaz, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 73a:** Assessing Discrepancies in Kinetic Parameters and Improving Combustion Models through Metaheuristic Optimization — **Nathan Harms**, *Sai Krishna Sirumalla, Richard H. West*

**8:22 Paper 73b:** Automated Discovery of Reaction Pathways for the Combustion of Alternative Fuel Candidates — **Ahmed E. Ismail**

**8:44 Paper 73c:** A Computational Investigation into the Kinetics of NO + CH<sub>2</sub>CCH and Its Effect on NO Reduction — **Aaron Danilack**, *C. Franklin Goldsmith*

**9:06 Paper 73d:** Diluent Effect on NO<sub>x</sub> Formation in Pressurized Combustion of Syngas/Air — **Nazli Asgari**, *Ryan Cichowicz, Bihter Padak*

**9:28 Paper 73e:** Ash Partitioning and Ultrafine Aerosol Formation Mechanism for Air and Oxy-Combustion of Coal, Biomass and Blends — **Yueming Wang**, *Xiaolong Li, Jost O. L. Wendt*

**9:50 Paper 73f:** Effect of SO<sub>2</sub> on CuMn<sub>2</sub>O<sub>4</sub> Oxygen Carrier's Reactivity for Chemical Looping with Oxygen Uncoupling (CLOU) — **Turna Barua**, *Sam Horlick, Bihter Padak*

**10:12 Paper 73g:** Simultaneous Removal of Hg(0) and NO over Modified SCR Catalyst — **Can Li**, *Zhouyang Liu, Vishnu Sriram, Joo-Youp Lee*

## (74) Computational Studies of Self-Assembly

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 307

Sumit Sharma, Chair  
Julia Dshemuchadse, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**8:00 Paper 74a:** Programming Colloidal Assembly into Aggregates and Crystals By Landscape Engineering — **Yutao Ma**, *Andrew W. Long, Andrew L. Ferguson*

**8:15 Paper 74b:** Symmetry-Based Discovery of Multicomponent, Two-Dimensional Colloidal Crystals — **Nathan A. Mahynski**, *Evan Pretti, Vincent K. Shen, Jeetain Mittal*

**8:30 Paper 74c:** Optimization of Smooth Isotropic Pair Potentials for the Self Assembly of Complex Structures — **Carl Simon Adorf**, *James Antonaglia, Julia Dshemuchadse, Sharon C. Glotzer*

**8:45 Paper 74d:** Structural Transformations in Binary Superlattices of DNA-Functionalized Particles — **Evan Pretti**, *Hasan Zerze, Yajun Ding, Minseok Song, Jeetain Mittal*

**9:00 Paper 74e:** Engineering Entropic Self-Assembly of Faceted Nanoparticles — **Abhishek K. Sharma**, *Vikram Thapar, Fernando A. Escobedo*

**9:15 Paper 74f:** FCC-to-BCC Phase Transitions of Convex and Concave Particles — **Duanduan Wan**, *Chrisy Xiyu Du, Greg van Anders, Sharon C. Glotzer*

**9:30 Paper 74g:** Unusual Crystallization Behavior Close to the Glass Transition — **Caroline Desgranges**, *Jerome Delhommelle*

**9:45 Paper 74h:** Elucidating a Network of Interactions That Drive Large-Scale and Pleomorphic Protein Assemblies during Viral Budding — **Alexander J. Pak**, *John M. A. Grime, Gregory A. Voth*

**10:00 Paper 74i:** Toward a Computational Protocol for the Design of Functional Amyloid Peptide Self-Assembling Materials — **Sai Vamshi R Jonnalagadda**, *Asuka A. Orr, Joseph M. Jakubowski, Kendal J. Henderson, Chang-Hyun Choi, Chrysoula Kokotidou, Anna Mitraki, Hae-Kwon Jeong, Phanourios Tamamis*

**10:15 Paper 74j:** On the Interplay between Conformational Complexity, Solution Structure, and Polymorphism in Succinic Acid Nucleation from Solution. — *Ilaria Gimondi, Matteo Salvai*

#### (75) Design, Construction, and Operation of Unit Operations Labs and Pilot Plants

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 336

Michael Trainor, Chair  
Vinod Kumar Venkatakrishnan, Co-Chair

**Sponsored by:** Pilot Plants

**8:00 Paper 75a:** Design, Construction and Operation of a Heat Exchanger Test Bed Unique for Leaks Detection and Modeling — *Daniel Chen, Dan Fernandes, Tae Hoon Kim*

**8:25 Paper 75b:** Design of a Test Rig for the Simulation of Startup Procedures in Main Heat Exchangers of Air Separation Plant — *Patrick Haider, Pascal Freko, Stefan Lochner, Thomas Reiter, Sebastian Rehfeldt, Harald Klein*

**8:50 Break**

**9:15 Paper 75d:** Syngas Chemical Looping and Coal Direct Chemical Looping Processes for Hydrogen and Power Production with in-Situ Carbon Capture: Pilot Scale Development and Demonstration — *Andrew Tong, Yitao Zhang, Sourabh Nadgouda, Tien-Lin Hsieh, Dawei Wang, Cheng Chung, Yaswanth Pottimurthy, Thomas Flynn, Luis G. Velazquez-Vargas, Liang-Shih Fan*

#### (76) Division Plenary: CAST (Invited Talks)

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 407

Carl D. Laird, Chair  
Prodromos Daoutidis, Co-Chair

**Sponsored by:** Computing Systems and Technology Division

**8:00 Paper 76f:** Overview of CAST Activities and Programming — *Carl D. Laird, Prodromos Daoutidis*

**8:15 Paper 76a:** Verifying Performance Specifications for Dynamic Processes Under Uncertainty Using Backward Reachability Analysis — *Kai Shen, Xuejiao Yang, Joseph Scott*

**8:42 Paper 76b:** An Embedded Model Predictive Controller for a Medical Oxygen Concentrator Device — *Matthew Ulrich, Rama Rao Vemula, Mayuresh V. Kothare*

**9:09 Paper 76c:** Online Scheduling Design Principles — *Dhruv Gupta, Christos T. Maravelias*

**9:36 Paper 76d:** Demand Response-Oriented Modeling and Production Scheduling Optimization for Chlor-Alkali Processes — *Joannah Otashu, Michael Baldea*

**10:03 Paper 76e:** Forty Years of Computers and Chemical Engineering (1977-2017): Analysis of the Field Via Natural Language Processing Techniques — *Tong Zhang, Nick Sahinidis, Carolyn Rose, Satyajith Amaran, Bo Shuang*

#### (77) Division Plenary: Gerhold and Kunes Awards on Separations (Invited Talks)

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 301

Roger D. Whitley, Chair  
Mark M. Davis, Co-Chair

**Sponsored by:** Separations Division

**8:00 Paper 77a:** Porous Crystalline Molecular Sieve Membranes for Kr/Xe Separation — *Moises Carreon*

**8:30 Paper 77b:** 3D Printing Thin Film Composite Membranes — *Magdud R. Chowdhury, Jeffrey R. McCutcheon*

**9:00 Paper 77c:** Bio-Inspired Low Biofouling Nanocomposite Membranes: From Batch-Scale to Continuous-Scale Membrane Fabrication — *Isabel Escobar*

**9:30 Paper 77d:** Enabling Widespread Use of Microporous Membranes for Challenging Organic Solvent Separations — *Ryan Lively*

**10:00 Paper 77e:** Batch Distillation Simulation, Optimization, and Control: Past, Present, and Future — *Urmila M. Diwekar*

#### (78) Effective Classroom and Laboratory Demonstrations

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 406

Jennifer Pascal, Chair  
Bradley C. Bundy, Co-Chair

**Sponsored by:** Undergraduate Education

**8:00 Paper 78a:** Fluidization Experiments in a Unit Operations Laboratory — *John Clay*

**8:18 Paper 78b:** Propagation of Hands-on Desktop Learning Pedagogy across Institution and Program Types — *Kitana M. Kaiphanliam, Negar Beheshti Pour, Aminul Islam Khan, Bernard J. Van Wie, David B. Thiessen, Prashanta Dutta, Robert F. Richards, Shamus Fanhe Meng*

**8:36 Paper 78c:** Design of an Automated Control System for a Continuous Distillation Column and Its Implementation into the Unit Operations Laboratory Experimental Program — *Patrick L. Mills, Alexander Jess, Brian West*

**8:54 Paper 78d:** Process Control Laboratory on Arduino and Simulink Platform — *Sohrab Rohani, Yuanyi Wu*

**9:12 Paper 78e:** Experimental System and Process Data Describing Model-Based Control Strategies in the Chemical Engineering Curriculum — *Doug Kelley, Eldred Chimowitz*

**9:30 Paper 78f:** Creative Student Activities to Enhance Teaching on Heat and Mass Transport — *Dimitrios V. Papavassiliou*

**9:48 Paper 78g:** Chemical Engineering 'on-a-Chip': Capturing the Integrated Scope of Chemical Engineering in a Single STEM Module — *Kelly M. Schultz, Mark A. Snyder*

**10:06 Paper 78h:** The Use of Numerical Worksheets in Undergraduate Courses — *Satish Parulekar*

#### (79) Electrocatalysis and Photoelectrocatalysis I: Fundamentals of CO<sub>2</sub> Reduction

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 401

Feng Jiao, Chair  
Michal Bajdich, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 79a:** Experimental and Theoretical Studies of the Electrochemical Reduction of CO<sub>2</sub> on Cu — *Alexis T. Bell*

**8:20 Paper 79b:** Highly Efficient CO Electroreduction Catalyst Based on Polycrystalline Cu Particles — *Jing Li, Qi Lu*

**8:40 Paper 79c:** Operando Spectroscopic Investigations of Oxide Derived Metal Catalysts for CO<sub>2</sub> and CO Reduction — *Arnav Malkani, Marco Dunwell, Bingjun Xu*

**9:00 Paper 79d:** Molecular-Level Insights into Electrocatalytic Carbon Dioxide Reduction at Cobalt Macrocycles — *Karthish Manthiram*

**9:20 Paper 79e:** Mass Transfer Effects in CO<sub>2</sub> Reduction Electrocatalysis — *Chao Wang*

**9:40 Paper 79f:** Single Atom Catalysts for Electrochemical Reduction of CO<sub>2</sub> — *Aditya Prajapati, Songwei Che, Vikas Berry, Meenesh R. Singh*

**10:00 Paper 79g:** Photoelectrochemical CO<sub>2</sub> Reduction at Plasmonic Nanostructured Silver Electrodes — *Elizabeth R. Corson, Erin B. Creel, Youngsang Kim, Matthew J. Liu, Davis D. Perez, Jeffrey J. Urban, Robert Kostecki, Bryan D. McCloskey*

#### (80) FEW Nexus: Emerging Chemical Engineering Innovations from Micro-Scale Innovations to Complex, Interconnected Systems (Invited Talks)

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 317

Fengqi You, Chair  
Dale Kearns, Co-Chair  
Nada Marie Anid, Co-Chair  
Leslie M. Shor, Co-Chair

**Sponsored by:** The Food-Energy-Water Nexus

**8:00 Welcoming Remarks**

**8:05 Paper 80a:** Food-Energy-Water Nexus Systems Engineering — *Efstathios N. Pistikopoulos, Richard Allen, Yaling Nie, Styliani Avraamidou*

**8:25 Paper 80b:** Overcoming Potential Land Constraint for Meeting Food, Energy and Water Needs in a Solar Economy — *Rakesh Agrawal*

**8:45 Paper 80c:** Opportunities for Sustainable Management of Dairy and Food Wastes Using Hydrothermal Thermal Processing to Recover Energy, Nutrients, and Clean Water — *Jefferson W. Tester*

**9:05 Paper 80d:** Renewable Carbons from Food Waste for Separation and Catalysis Technologies — *Julia A. Valla, Yu Lei, David P. Gamliel*

**9:25 Paper 80e:** A Computational Framework for Sustainable Waste Management and Simultaneous Recovery of Nutrients and Energy — *Gerardo J. Ruiz-Mercado, Victor M. Zavala, Mariano Martin*

**9:45 Paper 80f:** Recovery of Manufacturing Sectors in Puerto Rico Post-Hurricane Maria: FEW Nexus Findings and Opportunities — **Jennifer Helgeson, Ramon Vega-Alejandra, Migdalia Rosado-Garcia, Robert S. Weber, José Colucci**

**10:05 Paper 80g:** Nexus Integration: An Energy-Water Prototype Model — **Charles Zelek**

**10:25 Paper 80h:** An Engineer's Roadmap on Hurricane Infrastructure Resilience — **Michelle Bryner**

**10:30** Concluding Remarks

**(81) Forum Plenary: Pharmaceutical Discovery, Development, and Manufacturing Forum (Invited Talks)**  
**Monday, Oct 29, 8:00 AM**  
Westin Convention Center, Allegheny Grand Ballroom II

Jonathan McMullen, Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**8:00** Introductory Remarks

**8:10 Paper 81a:** Engineering Biocatalytic Cascades for the Production of Pharmaceuticals — **Matthew Truppo**

**8:55 Paper 81b:** Advanced Design of Experiment Methodologies for Enhanced Process Understanding — **Christos Georgakis**

**9:40 Paper 81c:** Continuous Processing for the Manufacture of Drug Substance — **Martin Johnson, Carla Luciani, Scott A. May, Kevin P. Cole**

**(82) Free Forum on Engineering Education: First Year and Sophomore Year**

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 411

Christi Patton Luks, Chair  
Jonathan Wenzel, Co-Chair

**Sponsored by:** Undergraduate Education

**8:00 Paper 82a:** Active Learning in a Large Lecture Setting Enhances Introductory Course — **Marjorie S. Went**

**8:18 Paper 82b:** Peer Led Team Learning in Chemical Engineering — **Sandra L. Pettit**

**8:36 Paper 82c:** Teaching Students How to Learn: Blending Retrieval Practice with Team-Based Learning in a Material and Energy Balances Course — **Monica Lamm**

**8:54 Paper 82d:** A New Curriculum to Train Chemical Engineers to Solve 21st Century Grand Challenges — **Mohammad Zandi, Siddharth V. Patwardhan, Linda Kotta, James D. Litster**

**9:12 Paper 82e:** Using Online Survey Tools to Facilitate Classroom Discussion on Process Safety — **Reginald E. Rogers Jr.**

**9:30 Paper 82f:** Introducing Chemical Engineering to Prospective Engineers — **Michael Senra**

**9:48 Paper 82g:** Ten Years in the Trenches: An Updated Suite of Scenario-Based Academic Integrity Videos — **Adam Melvin, Lisa G. Bullard**

**10:06 Paper 82h:** Evaluation of Conceptual Testing Enhanced with Technical Writing and Just-in-Time Teaching — **Matthew Cooper, Ishan Joshipura, Lisa G. Bullard**

**(83) Fuel Cells, Electrolyzers, and Electrochemical Devices**  
**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 324

Julie N. Renner, Chair  
Maureen H. Tang, Co-Chair

**Sponsored by:** Transport and Energy Processes

**8:00 Paper 83a:** The Effect of Loading, Test Parameters, and Oxides on Electrolyzer-Catalyst Durability — **Bryan S. Pivovar, Shaun M. Alia**

**8:20 Paper 83b:** Alkaline Stable Sustainion® Anion Exchange Membrane for Electrolyzers and Fuel Cells — **Zengcai Liu, Hongzhou Yang, Syed Dawar Sajjad, Liang Zhu, Jerry Kaczur, Richard I. Masel**

**8:40 Paper 83c:** Thermodynamic Modeling of Electric Double Layer in Capacitive Deionization Cell Electrodes with Condensation Theory — **Yue Yu, Yuan Li, Chau-Chyun Chen**

**9:00 Paper 83h:** Development of Devices and Selective Catalysts for the Solar-Driven Reduction of CO<sub>2</sub> to fuels — **Marcel Schreier, Michael Grätzel, Yogesh Surendranath**

**9:20 Paper 83e:** *Ab-Initio* Investigation of Dimethyl Disulfide As an Additive for Lithium-Sulfur Batteries — **Ethan P. Kamphaus, Perla B. Balbuena**

**9:40 Paper 83f:** Atomic Layer Deposition of Protective Coatings on LiMn<sub>2</sub>O<sub>4</sub> Cathodes — **Robert Warburton, Lin Chen, Matthias J. Young, Jeffrey Elam, Jeffrey Greeley**

**10:00 Paper 83g:** Silicon Li-Ion Anode Materials Via Spray Drying and Magnesiothermic Reduction — **Zheng Yan, Juchen Guo**

**(84) Fundamental Research in Transport Processes**

**Monday, Oct 29, 8:00 AM**

Omni William Penn Hotel, Conference Center B

Sara Hashmi, Chair  
Joel L. Plawsky, Co-Chair

**Sponsored by:** Transport Processes

**8:00 Paper 84a:** Rip Currents in Microgravity — **Thao Nguyen, Joel L. Plawsky, Peter C. Wayner Jr.**

**8:18 Paper 84b:** Effect of Porosity on Thermal Transport in Nanoscale Systems — **Abhinav Malhotra, Martin Moldovan**

**8:36 Paper 84c:** A Vacuum Set-up for Fundamental Studies of Self- and Transport Diffusion in Porous Media — **Haiyue Yu, Marc-Olivier Coppens**

**8:54 Paper 84d:** Understanding Transport of Small Solutes in the Pores of a Nanostructured Lyotropic Liquid Crystal Membrane — **Benjamin J. Coscia, Michael Shirts**

**9:12 Paper 84e:** A MEMS Investigation of Osmotic Pressure-Driven Flows — **Winston Black II, Abraham D. Stroock**

**9:30 Paper 84f:** A Theory of Enzyme Chemotaxis: Comparison between Experiment and Model — **Farzad Mohajerani, Xi Zhao, Ambika Somasundar, Darrell Velegol, Ayusman Sen**

**9:48 Paper 84g:** Multicomponent Diffusion in Aqueous Nonionic Micellar Solutions with Decane — **Nathan P. Alexander, Stephanie R. Dungan, Ronald J. Phillips**

**10:06 Paper 84h:** Internal Hydraulic Jump and Drop in Two Phase Gas-Liquid Flow over an Obstacle — **Mrinmoy Dhar, Gargi Das, Prasanta Kumar Das**

**(85) Fundamentals and Applications of Flow Assurance**

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 305

Francisco Vargas, Chair

**Sponsored by:** Upstream Engineering and Flow Assurance Forum

**8:00 Paper 85i:** Mitigation of Asphaltene Deposition by Dead Oil Recycle — **Aisha T. Khaleel, Francisco Vargas**

**8:17 Paper 85b:** Kinetics Study of Asphaltenes Adsorption Onto Hydrophilic Solid Surfaces — **Fang Liu**

**8:34 Paper 85c:** The Effect of Cyclic Molecules on the Gelation Characteristics of Polydisperse n-Alkane Systems — **Michael Senra, Ruikun Sun**

**8:51 Paper 85d:** Removal of Asphaltene from Crude Oil through Electrodeposition Method — **Shunxiang Xia, Kostarelos Konstantinos**

**9:08** Break

**9:18 Paper 85e:** The Influence of the Reservoir Acidity on Asphaltenes Dissolution in Aromatic Solvent Using Microsystems with *in Situ* Spectroscopy — **Weiqi Chen, Priyanga Vashistha, Andrew Yen, Nikhil Joshi, Yogesh Kapoor, Ryan L. Hartman**

**9:35 Paper 85f:** Effects of the Presence of Water in Cold Restart of Waxy Oils — **Yichen Wang, Jules Magda, Milind Deo**

**9:52 Paper 85g:** Avoiding Flowline Plugging: Hydrates Pressure Drop Signature, Plugging Onset Prediction and Deposition Mechanism — **Ben Bbosa, Michael Volk**

**10:09 Paper 85h:** Existence of Supersaturation and Its Effect on Wax Deposition Behavior — **Sriram Ravichandran, Nagu Daraboina, Cem Sarica**

**(86) Fundamentals of Environmental Kinetics and Reaction Engineering**

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 320

John A. Posada, Chair  
Andres Argoti, Co-Chair

**Sponsored by:** Fundamentals

**8:00** Break

**8:21 Paper 86b:** Density Functional Theory Insights into Corrosion and By-Product Formation Caused By Drinking Water Disinfection — **Margaret M. Reuter, Christian M. Lastoskie**

**8:42 Paper 86c:** Parameter Estimation of a Model of Advanced Oxidation Processes — **Maria A. Abreu Zamora, Vinay Prasad, Antonio Carlos S. C. Teixeira, Galo A. C. Le Roux**

**9:03 Paper 86d:** Kinetics and CFD Model Validation for Combustion of Coal Char Using Cu-Based Chemical Looping with Oxygen Uncoupling (CLOU) Carriers — **Ward A. Burgess, Nicholas C. Means, Bret H. Howard, Mark W. Smith, Dushyant Shekhawat**



**9:24 Paper 86e:** Graphene Coated Nickel Foam - a Novel Electrode for Electroperoxone Treatment of Emerging Pharmaceutical Contaminants — **Ramya Srinivasan, Indumathi Nambi**

**9:45 Paper 86f:** Dependence of Photocatalytic Degradation Pathway on Surface Planes of a Catalyst: A Case of Diuron Degradation on ZnO — **Sutaporn Meephon, Thanyada Rungrotmongkol, Somchintana Puttamat, Varong Pavarajarn**

**10:06 Paper 86g:** The Formation of Peroxymonocarbonate (HCO<sub>4</sub>·) and Its Impact on the Degradation of Organic Contaminants during Hydrogen Peroxide (H<sub>2</sub>O<sub>2</sub>) *in Situ* chemical Oxidation (ISCO) — **Xuejing Yang**

### (87) Fundamentals of Fluidization

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 415

Mayank Kashyap, Chair  
Marc-Olivier Coppens, Co-Chair

**Sponsored by:** Fluidization and Fluid-Particle Systems

**8:00 Paper 87h:** SABIC YPA Talk —

**8:24 Paper 87a:** Effect of Cohesion on Gas Residence Time Distribution in Fluidized Beds — **Jari Kolehmainen, Ali Ozel, Yundi Jiang, Sankaran Sundaresan**

**8:42 Paper 87b:** Drag Models and Their Validation: Unanswered Questions from the Past and Targeting Future Validation — **Casey Q. LaMarche, Ben Freireich, Ray Cocco**

**9:00 Paper 87c:** Assessment of Mesoscale Solid Stress in Coarse Grid TFM Simulation of Geldart A Particles in All Fluidization Regimes — **Xi Gao, Tingwen Li, William A. Rogers**

**9:18 Paper 87d:** Structured Bubbling Fluidized Beds: Nucleation and Self-Arrangement Under Pulsation — **Victor Francia, Kaiqiao Wu, Marc-Olivier Coppens**

**9:36 Paper 87e:** Cluster-Induced Deagglomeration in Unbounded Fluidization of Cohesive Particles — **Peiyuan Liu, Christine M. Hrenya**

**9:54 Paper 87f:** Discrete Particle Model for Non-Spherical Large Objects in Dense Gas-Solid Flows — **Yuya Sakamoto, Takuya Tsuji, Kimiaki Washino, Toshitsugu Tanaka, Koshi Uemoto, Shusaku Harada, Shunsuke Kato, Jun Oshitani, Hirokazu Kajiwara, Kei Matsuoaka**

**10:12 Paper 87g:** Particle Velocity Distribution Function and the Non-Equilibrium Characteristics of Gas-Solid Flows — **Bidan Zhao, Junwu Wang**

### (88) High Pressure Phase Equilibria and Modeling

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 306

Aaron M. Scurto, Chair  
Christopher L. Kitchens, Co-Chair

**Sponsored by:** High Pressure

**8:00 Paper 88a:** Phase Behavior, Densities, and Viscosities of Propylene + Toluene and Ethylene + Toluene Mixtures at Temperatures to 580 K and Pressures to 70 Mpa — **Rajendar R. Mallepally, Babatunde A. Bamgbade, Nathaniel A. Cain, Mark A. McHugh**

**8:25 Paper 88b:** Estimation of the Density of CO<sub>2</sub>/Organic Solvent Systems with Peng-Robinson Equation of State — **Ken Kuwabara, Hiroaki Matsukawa, Yuichiro Shimada, Masakazu Naya, Atsushi Shono, Tomoya Tsuji, Katsuto Otake**

**8:50 Paper 88c:** Sanchez-Lacombe Parameters for Silicone Alkoxides — **Hiroaki Suzuki, Hiroaki Matsukawa, Yuichiro Shimada, Masakazu Naya, Atsushi Shono, Taka-aki Hoshina, Tomoya Tsuji, Katsuto Otake**

**9:15 Paper 88d:** Carbon Dioxide and Methane Mixture Adsorption on Clay Mineral Surfaces in the Presence of Residual Water Content: A Molecular Simulation Study — **Leebyn Chong, Dustin Crandall, Evgeniy M. Myshakin**

**9:40 Paper 88e:** Theoretical Investigation of Iron Spin Crossover Pressure in Fe-Bearing MgO — **Zhi Zeng, Xianlong Wang, Kaishuai Yang, Ya Chen, Jie Zhang**

### (89) In Honor of Doraiswami Ramkrishna's 80th Birthday I (Invited Talks)

**Monday, Oct 29, 8:00 AM**

Westin Convention Center, Somerset

Meenesh R. Singh, Chair  
Jamey D. Young, Co-Chair

**Sponsored by:** Food, Pharmaceutical & Bioengineering Division

**8:00** Introductory Remarks

**8:25 Paper 89a:** A Long Journey with Prof. Ramkrishna – from Modeling Mammalian Cells to Balancing Bacteria — **Wei-Shou Hu**

**8:50 Paper 89b:** Microbial Community Modeling: The Cybernetic Perspective — **Hyun-Seob Song**

**9:15 Paper 89c:** Computational Challenges in Systems Biology — **Shankar Subramaniam**

**9:40 Paper 89d:** The Value of Modeling in Cell Mechanics — **Tanmay Lele**

**10:05 Paper 89f:** Pore Formation by Antimicrobial Peptides in Cell Membranes — **Ganesan Narsimhan**

### (90) In Honor of Michael Smith's 60th Birthday I (Invited Talks)

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 405

Jeffrey Rimer, Chair  
Phillip Christopher, Co-Chair  
Michael A. Smith, Co-Chair  
Alexander Zoelle, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 90a:** Maximizing Efficiencies of Photocatalytic Water Splitting By Engineering Interfaces in Multi-Component Photocatalysts — **Suljo Linic**

**8:20 Paper 90b:** Recent Advances in Zeolite-Based Technologies — **Javier Guzman**

**8:40 Paper 90c:** Direct Synthesis of H<sub>2</sub>O<sub>2</sub> from H<sub>2</sub>/O<sub>2</sub> Mixtures and Its Decomposition over Intermetallic Pd-Zn Catalysts — **Tianze Xie, Anish Dasgupta, Robert Rioux**

**9:00 Paper 90d:** Oxygen Electrocatalysis Using Layered Mixed Metal Oxides — **Eranda Nikolla**

**9:20 Paper 90e:** Improved Carbon Coatings for Nitrogen Production and Upgrading Pyrolysis Oils — **Charles Coe**

**9:40 Paper 90f:** Hybrid Materials for Catalysis and Separations — **Daniel F. Shantz**

**9:55 Paper 90g:** Structural and Dynamic Characteristics of Supported Metal Catalysts at the Atomic Scale — **Phillip Christopher**

**10:10 Paper 90h:** Carbide-Based Electrocatalysts in Alkaline Electrolyte — **Jingguang G. Chen**

### (91) In Honor of Pablo Debenedetti I (Invited Talks)

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 308

M. Scott Shell, Chair  
Jean W. Tom, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**8:00 Paper 91a:** Introduction — **M. Scott Shell, Jean W. Tom**

**8:05 Paper 91b:** Pablo Debenedetti: Recollections from the Past 36 Years — **Athanassios Z. Panagiotopoulos**

**8:25 Paper 91c:** Pressure: The Neglected Variable in High Pressure Processing — **Keith E Gubbins, Kai Gu, Liangliang Huang, Yun Long, James Mansell, Erik E. Santiso, Kaihang Shi, Malgorzata Sliwinska-Bartkowiak, Deepti Srivastava**

**8:45 Paper 91d:** Polymer-Grafted Nanoparticle Membranes with Controllable Free-Volume — **Sanat K. Kumar**

**9:05 Paper 91e:** On the Thermodynamics of Systems Under the Influence of Gravity — **David S. Corti**

**9:25 Paper 91f:** Thermodynamics of Ionic Liquid Mixtures — **Joan F. Brennecke**

**9:45 Paper 91g:** Forward Flux Sampling Using Jumpy Order Parameters — **Amir Haji-Akbari**

**10:05 Paper 91h:** Machine Learning for Design and Detection of Assembly — **Thomas M. Truskett**

### (92) Integrating Municipal and Industrial Waste into Biorefineries

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 316

Emmanuel Revellame, Chair  
Chenlin Li, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**8:00 Paper 92a:** Hydrothermal Liquefaction of Municipal Solid Waste Using Binary Transition Metal Oxide (BTMO) Nanoparticles — **Vinod S. Amar, Anuradha Shende, Rajesh Shende**

**8:25** Break

**8:50 Paper 92c:** Economic and Environmental Sustainability of the Production of Chemicals from a Pyrolysis-Based High Density Polyethylene Refinery — **Ulises R. Gracida-Alvarez**, Olumide Winjobi, Julio C. Sacramento-Rivero, David R. Shonnard

**9:15 Paper 92d:** Insights into the Anaerobic Digestion of Catfish and Shrimp Processing Wastewaters — **Dhan Lord Fortela**, Emmanuel Revellame, Wayne Sharp, Mark Zappi

**9:40 Paper 92e:** Synthesis of a Sustainable Multifunctional Biodiesel Additive from Lipid-Enhanced Sludges — **Randy Maglinao**, Emmanuel Revellame

**(93) Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage**  
**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 318

Wei Liu, Chair  
Jian Liu, Co-Chair  
Anthony Shoji Hall, Co-Chair  
Yunfa Chen, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**8:00 Paper 93a:** Electrochemical Production of Ammonia from Nitrogen and Water for Electrical Energy Storage — **Wei Liu**, Anirudh Balram, Peipei Wang

**8:25 Paper 93b:** A Novel Binder to Improve the Electrochemical Performance of Si/C Anode of Lithium Batteries — **Liyuan Li**, Lan Zhang, Suojang Zhang

**8:50 Paper 93c:** Thermal Energy Storage (TES) with Silica Gel Regenerated at Low Temperature — **Ye Hua**, F. Handan Tezel

**9:15 Paper 93d:** Efficient Hydrogen Production from Solar Thermal Energy Via High Temperature Water Electrolysis — **Yiru Li**, Rakesh Agrawal

**9:40 Paper 93e:** Thermochemical Hydrogen Production Via  $\text{Ce}(\text{SO}_4)_2/\text{Ce}_2\text{O}_3$  Based  $\text{H}_2\text{O}$  Splitting Cycle — **Rahul Bhosale**, Gorakshnath Takalkar

**(94) Modeling of Particulate Systems**  
**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 414

Martin Pillei, Chair  
Kuo-Chen Tsai, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**8:00 Paper 94a:** Flow Behavior of Particulate Pine Forest Residues and Corn Stover: A Comparison of Experiments and Simulations — **Tyler L. Westover**, Yidong Xia, Kunal S. Pardikar, Jordan Klinger, Sergio Hernandez, Hai Huang, Carl Wassgren

**8:18 Paper 94b:** Flow Rate Interference Effects in a Silo with Two Openings — **Luke Fullard**, Eric Breard, Clive E. Davies, Jonathan Godfrey

**8:36 Paper 94c:** Dissolution of Polymer Particulate Systems: Population Ensemble Modeling — **Mohammad Ghasemi**, Marina Tsianou, Paschalis Alexandridis

**8:54 Paper 94d:** Benchmarking a Novel 0-D Model Against Data from Two-Fluid Model Simulations of a Wet Fluidized Bed — **Stefan Radl**, Maryam Askarishahi, Mohammad-Sadegh Salehi

**9:12 Paper 94e:** Scale up Studies of Dry Catalyst Impregnation for Improved Content Uniformity Using Simulations and Experiments — **M. Silvina Tomassone**, Yangyang Shen, William G. Borghard, Sai Sasidhar Guduru, Deval Sharma, Matthew Borsellino

**9:30 Paper 94f:** Dense Packing of Cell Monolayers: Jamming of Deformable Polygons — **Arman Boromand**, Corey S. O'Hern, Mark D. Shattuck, Fangyu Ye

**9:48 Paper 94g:** Blend Uniformity Prediction Based on Discrete Element Method — **Shuichi Tanabe**

**10:06 Paper 94h:** One-Way Coupled CFD-DEM Analysis of Particulate Flows in a Monodose Dry Powder Inhaler — **Yu Liu**, Ariel Muliadi, Lucilla Almeida, Carl Wassgren, Rahul Bharadwaj, Edward Yost, Ajit Narang

**(95) Molecular Simulation and Modeling of Complex Molecules**  
**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 309

Steven M. Abel, Chair  
Mohammadreza Samieegohar, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**8:00 Paper 95a:** Molecular Design of Polymer and Colloid By a Novel Solution Method Using Interfacial Statistical Associating Fluid Theory (iSAFT) — **Shun Xi**, Walter G. Chapman

**8:18 Paper 95b:** Coarse-Grained SAFT- $\gamma$  Force Fields for the Molecular Modelling of Resins and Asphaltenes — **Guadalupe Jiménez-Serratos**, George Jackson, Erich A. Müller, Tim Totton

**8:36 Paper 95c:** Designing of High- $\chi$  Block Oligomers for Assessing 1-Nm Domains and Understanding the Effects of Molecular Weight on  $\chi$  and the Effect of Dispersity on Blend Phase Diagrams — **Qile Chen**, Marc A. Hillmyer, Timothy P. Lodge, J. Ilja Siepmann

**8:54 Paper 95d:** Atomistic Simulation of Ionic Liquid Crystals — **Michael Quevillon**, Jonathan K. Whitmer

**9:12 Paper 95e:** Designing Molecular Building Blocks to Minimize Defects in the Formation of Surface Covalent Organic Frameworks — **Tiara Ann Maula**, Srinivas Rangarajan, Jeetain Mittal

**9:30 Paper 95f:** Mesoscale Modeling of Liquid-Liquid Solvent Extraction from Soft Matter Approach — **Anwesa Karmakar**

**9:48 Paper 95h:** Computational Modeling of RNA Aptamers: Structure Prediction of the Ligand-Free State — **Shuting Yan**, Muslum Ilgu, Marit Nilsen-Hamilton, Monica H. Lamm

**(96) Nanomaterials for Biological Application I**

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 412

Cerasela Zoica Dinu, Chair  
Jungbae Kim, Co-Chair

**Sponsored by:** Nanomaterials for Applications in Energy and Biology

**8:00 Paper 96a:** Invited Talk: Nanotherapeutics for Neuroprotection in the Developing Brain — **Elizabeth Nance**, Andrea Joseph, Rick Liao, Kylie Corry, Tommy Wood, Sandra Juul, Jessica Snyder, Pratik Parikh

**8:22 Paper 96b:** In Vivo Imaging of Larval Zebrafish Neurochemistry with Near-Infrared Dopamine Nanosensors — **Jackson Travis Del Bonis-O'Donnell**, Shih-Wei Chou, Irene Grossrubatscher, Ehud Isacoff, Markita Landry

**8:33 Paper 96c:** Functional Mesoporous Silica for Immunoengineering and Immunotherapy — **Jaeyun Kim**

**8:55 Paper 96d:** Biodegradable Interfacing Nanocomposite Coatings for Modulating the Cellular Response — **Valentina Dinca**, Laurentiu Rusen, Anisoara Campean

**9:06 Paper 96e:** Photo-Induced Polymerization and Reconfigurable Assembly of Multifunctional Ferrocene-Tyrosine — **Xuejiao Yang**, Yuefei Wang, Wei Qi

**9:17 Break**

**9:27 Paper 96f:** Green Synthesis of Fluorescent Nanomaterials for Optical Bioimaging and Beyond — **Dan Wang**, Yuan Pu, Jie-Xin Wang, Jian-Feng Chen

**9:45 Paper 96g:** Biological Self-Assembly and Recognition Used to Synthesize and Guide Next Generation of Hybrid Bio-Nano-Materials — **Xiao Hu**, Paolo Fagone, Chenbo Dong, Rigü Su, Quan Xu, Cerasela Zoica Dinu

**10:03 Paper 96h:** A Model-based Analysis of the Tissue-Targeting Efficacy of Ligand-Directed Nanoparticles — **Mohammad Aminul Islam**, Dipak Barua

**10:14 Paper 96i:** Pendant HDAC Inhibitor SAHA Derivatized Polymer As a Novel Prodrug Micellar Carrier for Anticancer Drugs — **Jieni Xu**

**10:25 Paper 96j:** Iron Sulfide Supraparticles As Artificial Viruses for Gene and Gene Editing Therapies — **Emine S. Turali-Emre**, Ahmet Emre, Nicholas Kotov

**(97) National Student Paper Competition**

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 410

William G. Pitt, Chair  
Douglas Ludlow, Co-Chair

**Sponsored by:** Student Chapters Committee Liaison

**8:00 Welcoming Remarks**

**8:05 Paper 97a:** Prediction of Optimal Chemotherapy Dosing Regimens: Balancing Tumor Degradation and Toxicity Effects — **Ian Dunn**, Kirti M. Yenkie

**8:20 Paper 97b:** Effects of Waste Vegetable Oil in High Concentration Recycled Asphalt Pavement Binder Mixes — **Connor Dugan**, Edgar A. O'Rear, Shivani Rani, Ashik Ali, Musharraf Zaman

**8:35 Paper 97c:** Microfluidic Modulation of Neural Differentiation of 3D Stem Cell Aggregates — **Amanda W. Schaefer**, Emily L. Jackson-Holmes, Todd McDevitt, Hang Lu



**8:50 Paper 97d:** Building Better Proteins: Integrating Cell-Free Protein Synthesis and Coarse-Grained Molecular Simulation to Rapidly Determine the Optimal Location for PEGylation — **Joshua W. Wilkerson**, *Kristen M. Wilding, Addison K. Smith, Derek B. Bush, Thomas A. Knotts IV, Bradley C. Bundy*

**9:05 Paper 97e:** Anionic Microgels for the Trypsin-Mediated Retention and Release of Therapeutic Proteins — **Joann Gu**, *John R. Clegg, Nicholas A. Peppas*

**9:20** Break

**9:30 Paper 97f:** Desktop Learning Modules (DLMs) and Their Effects on Student Progression through Bloom's Taxonomy for Fluid Mechanics Concepts — **Kitana M. Kaiphanliam**, *Negar Beheshtipour, Bernard J. Van Wie, David B. Thiessen*

**9:45 Paper 97g:** Characterization of Polymer Binders to Improve Cyclability of Lithium-Sulfur Batteries — **Richard Sim**

**10:00 Paper 97h:** Efficient Coacervate Extraction of Cationic Industrial Dye from Wastewater — **Benjamin Valley**, *Benxin Jing, Yingxi Elaine Zhu*

**10:15 Paper 97i:** Estimation of Critical Exponents Using Asymptotic Approximants — **Logan Melican**

#### (98) Novel and Unconventional Mixers

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 334

Laura J. Dietsche, Chair  
Sanja Miskovic, Co-Chair

**Sponsored by:** North American Mixing Forum

**8:00 Paper 98a:** Mixing Efficiency in a Simple, Continuous, Laminar-Flow Microdevice Using Computational and Experimental Approaches — **Siril Arockiam**, *Sagnik Basuray, Piero M. Armenante*

**8:30 Paper 98b:** Effect of Shear Gap Width on Flow and Power Draw in an Inline Rotor-Stator Mixer — **Kanan Ghaderzadeh**, *Richard V. Calabrese*

**9:00 Paper 98c:** Comparison of Breakup Kernels in the CFD-PBM Simulation of a Pulsed Disc and Doughnut Column — **Xiong Yu**, *Shan Jing, Shaowei Li*

**9:30 Paper 98d:** Performance Characterization of the GS-4 Gas Induction Impeller — **Kevin Myers**, *Shannon M. Hoffman, Eric E. Janz*

**10:00 Paper 98e:** The Effect of Scale-up on Mixing Efficiency in Oscillatory Flow Reactors Using Principal Component Based Analysis As a Novel Residence Time Distribution Measurement Tool — **Joseph Oliva**, *Botond Szilagyi, Zoltan K. Nagy*

#### (99) Novel Complex Flows (Invited Talks)

**Monday, Oct 29, 8:00 AM**  
Omni William Penn Hotel, Frick

Vivek Sharma, Chair  
Sujit S. Datta, Co-Chair

**Sponsored by:** Fluid Mechanics

**8:00 Paper 99a:** Formation and Disruption of a Particle Coating on a Confined Bubble — **Charles Sharkey**, *Zixian Cui, Shelley L. Anna*

**8:30 Paper 99b:** New Twists in the Electrohydrodynamics of Viscous Drops — **Petia M. Vlahovska**

**9:00 Paper 99c:** The Pulse of Plants — **Abraham D. Stroock**

**9:30 Paper 99d:** Life in Complex Fluids — **Paulo E. Arratia**

**10:00 Paper 99e:** Multiflagellarity Stabilizes Bacterial Locomotion Against Buckling — **Michael D. Graham**

#### (100) Process Research for Improved Throughput & Efficiency, and Reduced Cost & Environmental Impact

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 335

Rob Nunley, Chair  
Ida Chen, Co-Chair

**Sponsored by:** Process Research and Innovation

**8:00 Paper 100a:** Monitoring and Classification System for Water Recycling — **Ted J. Amundsen**, *Andrew L. Wagner*

**8:25 Paper 100b:** Water Recovery and Reuse in Soluble Coffee Production Using a Dynamic Membrane Process — **C. Stewart Slater**, *Mariano J. Savelski, Christian Wisniewski*

**8:50 Paper 100c:** How Active Is Too Active? a Catalyst Selection Study — **Dylan Kipp**, *Curtis Carlson, Daniel Martenak, Okiki Olufokunbi*

**9:15 Paper 100d:** Glycol Loss Minimization for a Natural Gas Dehydration Plant Under Upset Conditions — **Md Emdadul Haque**, *Srinivas Palanki, Qiang Xu*

**9:40 Paper 100e:** Hydrodeoxygenation of Karanja Oil for the Production of Green Diesel: Process Design with Heat Integration and Economic Analysis — **Swarnalatha Mailaram**, *Sunil Kumar Maity*

**10:05 Paper 100f:** An Integrated Process for Desulfurization (HDS-Extractive-Oxidative) — **Mohammad Reza Dehghani**, *Farhad Banisharif, Mahsa Mokhtarian*

#### (101) Rational Catalyst Design I

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 403

Adam Holewinski, Chair  
Jean-Sabin McEwen, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 101a:** Earth Abundant Perovskite Oxides for Low Temperature CO<sub>2</sub> Conversion — **Debtanu Maiti**, *Bryan J. Hare, Adela E. Ramos, Yolanda A. Daza, John N. Kuhn, Venkat R. Bhethanabotla*

**8:20 Paper 101b:** Rationalizing the Reactivity of Bimetallic Molecular Catalysts for CO<sub>2</sub> Hydrogenation — **Jingyun Ye**, *Ryan C. Cammarota, Jing Xie, Matthew Vollmer, Laura Gagliardi, Connie C. Lu, Christopher Cramer, Donald G. Truhlar*

**8:40 Paper 101c:** Physical Descriptors That Control Metal-Support Interactions Identified with DFT and Statistical Learning — **Thomas P. Senftle**

**9:00 Paper 101d:** Examining Acid Formation during the Selective Dehydration of Fructose to 5-Hydroxymethylfurfural in DMSO and Water — **Mariah Whitaker**, *Aamena Parulkar, Rutuja Joshi, Nicholas Brunelli*

**9:20 Paper 101e:** Does Hydrophobic Modification of Solid Acid Catalysts Promote Water Tolerance during Condensed Phase Catalytic Reactions of Oxygenates? — **William Elliott**, *Yanyu Mu, Isabel Burgos, Joann Sutyak, Robert M. Rioux*

**9:40 Paper 101f:** Designing Immobilized Tertiary Amine Catalysts for Selective Isomerization of Glucose to Fructose — **Nitish Deshpande**, *Lagnajit Pattanaik, Mariah Whitaker, Chi-Ta Yang, Li-Chiang Lin, Nicholas Brunelli*

**10:00 Paper 101g:** Supported Gold Clusters with Modulated Environment for Catalysis — **Nidhi Kapil**, *Michael M. Nigra, Marc-Olivier Coppens*

#### (102) Reaction Engineering in Pharmaceuticals and Fine Chemicals

**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 404

Anuj A. Verma, Chair  
Gaurav Giri, Co-Chair  
Marimuthu Andiappan, Co-Chair  
Ali Rowanaghi, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 102a:** In-Flow Production of Levoglucosenone from the Catalytic Dehydration of Cellulose Using Homogeneous Brønsted Acid Catalysts in  $\gamma$ -Valerolactone — **Alexa M. González-Rosario**, *Oscar Oyola-Rivera, Nelson Cardona-Martínez*

**8:15 Paper 102b:** Cyclooctene Cooxidation-Facilitated Co-ZSM-5-Catalyzed Selective Oxidation of Ethylbenzene with Molecular O<sub>2</sub> — **Anyang Peng**, *Matthew Ross, Linping Qian, Mayfair C. Kung, Brian Hoffman, Harold H. Kung*

**8:30 Paper 102c:** Dirhodium Immobilized Hollow Fiber Flow Reactor for Scalable and Sustainable C-H Functionalization in Continuous Flow — **Chun-Jae Yoo**, *Daniel Rackl, Wenbin Liu, Caroline Hoyt, Brian R. Pimentel, Ryan Lively, Huw M. L. Davies, Christopher W. Jones*

**8:45 Paper 102d:** Catalytic Dehydration of Levoglucosan and Cellulose to Levoglucosenone Using Brønsted Solid Acid Catalysts in Tetrahydrofuran — **Oscar Oyola-Rivera**, *Jiayue He, George W. Huber, James A. Dumesic, Nelson Cardona-Martínez*

**9:00 Paper 102e:** Composite Hollow Fiber Microfluidic Catalytic Reactors for Direct Conversion of Glucose to 5HMF — **Yingxin He**, *Fateme Rezaei, Ali Rowanaghi*

**9:15 Paper 102f:** Water Soluble Palladium- $\beta$ -Cyclodextrin Complex and Its Catalytic Performance for a Suzuki-Miyaura Cross-Coupling in Flow — **Yukun Liu**, *Ryan L. Hartman*

**9:30 Paper 102g:** Regioselective Epoxide Ring Opening with Alcohols Using Heterogeneous Lewis Acid Catalysts — **Nitish Deshpande**, *Nicholas Brunelli, Aamena Parulkar, Rutuja Joshi, Alexander Spanos*



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AIChEEvents app.

### (103) Redox Flow Batteries for Energy Storage

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 323

Jason Morgan, Chair

**Sponsored by:** Transport and Energy Processes

**8:00 Paper 103a:** The Influence of Electrode Microstructure on the Performance of Non-Aqueous Redox Flow Batteries — **Antoni Forner-Cuenca**, Emily Penn, Alexandra Oliveira, Fikile Brushett

**8:18 Paper 103b:** Method for Rapid Evaluation of Graphite Felt Electrode Stability in Vanadium Redox Flow Battery — **Jaromir Povedic**, Petr Mazur, Jindřich Mrlík, Jiri Vrana, Jan Dundalek, Juraj Kosek

**8:36 Paper 103c:** Designing Electrocatalysts for Vanadium-Based Flow Batteries for Renewable Energy Storage — **Nirala Singh**, Harsh Agarwal, Jin-Xun Liu, Bryan Goldsmith

**8:54 Paper 103d:** Increasing the Charge Storage Capacity of Phenothiazine-Based Electrolytes for Nonaqueous Redox Flow Batteries — **Jeffrey A. Kowalski**, N. Harsha Attanayake, Susan A. Odom, Fikile Brushett

**9:12 Paper 103e:** Investigating Cyclability of Aqueous Redox Flow Battery Electroactive Species at High Concentrations — **Scott L. A. Johnson**, Levi T. Thompson

**9:30 Paper 103f:** Systems Approaches to Predict the Aqueous Solubility of Quinone Molecules for Flow Battery Applications — **Sivadurgaprasad Chinta**, Raghunathan Rengaswamy

**9:48 Paper 103g:** A Novel Sulfonated Aromatic Polymer Membrane with Different Pendant Groups for Vanadium Redox Flow Batteries (VRFBs) — **Tongshuai Wang**, Junyoung Han, Kihyun Kim, Jannice Lee, Chulsung Bae, Sangil Kim

**10:06 Paper 103h:** Understanding the Influence of Thermal Pretreatment on Carbon Paper Electrodes for Vanadium Redox Flow Batteries — **Katharine V. Greco**, **Antoni Forner-Cuenca**, Fikile Brushett

### (104) Stem Cell and Tissue Engineering I: Engineering Cells

**Monday, Oct 29, 8:00 AM**

Westin Convention Center, Butler

Ipsita Banerjee, Chair  
Yuguo Lei, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**8:00 Paper 104a:** NANOG Restores Collagen Type III Production in Aged Stem Cells — **Na Rong**, Panagiotis Mistriotis, Xiaoyan Wang, Georgios Tseropoulos, Nika Rajabian, Stelios T. Andreadis

**8:18 Paper 104b:** A Physiologically Relevant Microenvironments for the Scalable Biomanufacturing Human Pluripotent Stem Cells — **Qiang Li**, Haishuang Lin, Ou Wang, Yuguo Lei

**8:36 Paper 104c:** Developmentally Inspired Hepatic Organoids Derived from Human Pluripotent Stem Cells — **Ogechi Ogoke**, Cortney Ott, Allison Kalinousky, Tala Mon, Natesh Parashurama

**8:54 Paper 104d:** Alginate Encapsulation for Large Scale Human Pluripotent Stem Cell Production — **Connor Wiegand**, Bo Lin, Thomas Richardson, Joseph E. Candiello, Ipsita Banerjee

**9:12 Paper 104e:** Decoy TRAIL Receptor CD264: A Predictor of in Vitro Regenerative Potential for Mesenchymal Stem Cells — **Sean Madsen**, Katie Russell, Alan Tucker, Julie Glowacki, Bruce Bunnell, Kim O'Connor

**9:30 Paper 104f:** Visualizing the Heterogeneity within Primary Hematopoietic Cell Populations with Self-Organizing Maps of Secondary Ion Mass Spectrometry Data — **Vahid Mirshafiee**, Brendan A. Harley, Mary L. Kraft

**9:48 Paper 104g:** Invited Speaker: The Impact of Physicochemical Cues during Vascular Differentiation and Morphogenesis — **Sharon Gerecht**

### (105) Student Design Competition

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 409

Sarah Ewing, Chair

**Sponsored by:** Student Chapters Committee Liaison

### (106) Teaching with Technology

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 408

Matthew Cooper, Chair  
Monica Lamm, Co-Chair

**Sponsored by:** Education

**8:00 Paper 106a:** Developing Engineering Thinking during an Ill-Structured Activity for Kinetics and Reactor Design: A Technology Solution — **Milo D. Koretsky**, James L. Gugel, Thomas Ekstedt

**8:18 Paper 106b:** Reading and Repetition Using an Interactive Textbook for Material and Energy Balances — **Matthew Liberatore**, Katherine Roach

**8:36 Paper 106c:** Check Your Homework with Your Phone — **John Wagner**, Amanda P. Malefyt, Garth Thomas Jr.

**8:54 Paper 106d:** Educational Augmented Reality Tools: Development, Implementation, and Assessment of Phase I — **Konstantinos E. Kakosimos**, Ghada Salama, Marcelo Castier, Marcin Kozusznik

**9:12 Paper 106e:** Preparing Chemical Engineering Students for the Digitalization of Tomorrow – Integrating Modelling across the Curriculum — **Eva Sorensen**, Pieter Schmal

**9:30 Paper 106f:** Wastewater Minimization and Energy Conservation Software Developed and Used in Teaching Process Systems Engineering at Vanderbilt — **Russell F. Dunn**, Scott A. Guelcher, Bryan Beyer

**9:48 Paper 106g:** Aspen Plus® Videos for Chemical Engineering Undergraduates — **Michael Shao**, Mark B. Shiflett, Alejandra Rocha

**10:06 Paper 106h:** Problem Solving Skills When Using Student-Generated Problems That Reverse Engineer YouTube Videos — **Uchenna Asogwa**, Amanda P. Malefyt, T Ryan Duckett, Gale Mentzer, Charlene Czerniak, Matthew Liberatore

### (107) Topical Plenary: Microbial Interaction with Biointerfaces (Invited Talks)

**Monday, Oct 29, 8:00 AM**

Westin Convention Center, Pennsylvania East

Kenneth Urish, Chair  
Pushkar Lele, Co-Chair

**Sponsored by:** Microbes at Biomedical Interfaces

**8:00 Paper 107a:** Bad to the Bone: Biofilm and Surgical Infection — **Kenneth Urish**

**8:25 Paper 107b:** The Microbiome in Health and Disease — **Alison Morris**

**8:50 Paper 107c:** Viable but Non-Culturable and Persistence Describe the Same Bacterial Stress State (invited talk) — **Thomas K. Wood**

**9:15 Paper 107d:** Evolution of Nitric Oxide Resistance in *Staphylococcus Aureus* — **Anthony Richardson**

**9:40 Paper 107e:** Mechano-Morphogenesis and the Capillary Peeling of Biofilms — **Howard A. Stone**

### (109) Young Professional Research Projects in Industry (Invited Talks)

**Monday, Oct 29, 8:00 AM**

David L. Lawrence Convention Center, 303

Kartik Bomb, Chair  
Srihari K. Maganti, Co-Chair

**Sponsored by:** Young Professionals Committee (YPC)

**8:00 Paper 109a:** Supercritical Impregnation of Walnut Husk Extract into Polyethylene Film — **Isaiah Spencer-Williams**

**8:25 Paper 109b:** Improved Octane Barrel Recovery — **Prajwal Shinde**

**8:50 Paper 109d:** Reductive loop swaps in polyketide synthases as a route to designer chemical products — **Ravi Lal**

**9:15 Break**

**9:40 Paper 109e:** Soft film delamination from dynamic wrinkling substrates — **Joseph Hamm**

**10:05 Paper 109f:** Transitioning from Batch to Flow: Microbial Fuel Cells for Saline Wastewater Treatment — **Stuart Robertson**

### (110) Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks)

**Monday, Oct 29, 8:30 AM**

David L. Lawrence Convention Center, 310

Geoffrey D. Bothun, Chair  
Reginald E. Rogers Jr., Co-Chair

**Sponsored by:** Nanoscale Science and Engineering Forum

**8:30 Paper 110a:** Forum Award Winner — **Sharon C. Glotzer**

**9:30 Paper 110b:** Young Investigator Award - Nanotechnology As a Tool to Study and Direct Immune Function — *Christopher M. Jewell*

**(111) Microbes at Biomedical Interfaces Undergraduate Poster Competition**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Tagbo H.R. Niepa, Chair  
Jackie Shane, Co-Chair

**Sponsored by:** Annual Student Conference

**(112) Undergraduate Student Poster Session: Catalysis and Reaction Engineering**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(113) Undergraduate Student Poster Session: Computing and Process Control**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(114) Undergraduate Student Poster Session: Education & General Papers**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(115) Undergraduate Student Poster Session: Environmental**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(116) Undergraduate Student Poster Session: Food, Pharmaceutical, and Biotechnology**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(117) Undergraduate Student Poster Session: Fuels, Petrochemicals, and Energy**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(118) Undergraduate Student Poster Session: Materials Engineering and Sciences**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(119) Undergraduate Student Poster Session: Separations**

**Monday, Oct 29, 10:00 AM**  
David L. Lawrence Convention Center, Exhibit Hall B

Victor Breedveld, Chair

**Sponsored by:** Annual Student Conference

**(120) The Future of Energy in the Region, Nation and World (Invited Talks)**

**Monday, Oct 29, 11:00 AM**  
David L. Lawrence Convention Center, Spirit of Pittsburgh B

J. Karl Johnson, Chair  
Cliff Kowall, Co-Chair

**Sponsored by:** Miscellaneous

**11:00 Paper 120b:** 2018 Outlook for Energy: A View to 2040 — *Theodore J. Wojnar Jr.*

**11:20 Paper 120c:** Energy Decarbonisation Scenarios — *Kamel Ben Naceur*

**11:40 Paper 120a:** Fundamental Research Needs to Advance Energy Technologies — *Bruce Garrett*

**12:00** Panel Discussion

**(121) 2018 Danckwerts Lecture**

**Monday, Oct 29, 11:15 AM**  
Westin Convention Center, Allegheny Grand Ballroom II

Anton P. J. Middelberg, Chair

**Sponsored by:** Awards Committee

**11:15 Paper 121a:** Biotechnology to Help Achieve the UN's Sustainable Development Goals — *Sang Yup Lee*

**(122) WIC Luncheon (Ticketed Event) Monday, Oct 29, 11:00 AM**

David L. Lawrence Convention Center, Spirit of Pittsburgh A

Shannon L. Servoss, Chair  
Bindu Krishnan, Co-Chair

**Sponsored by:** Women's Initiatives Committee (WIC)

**11:00** Panel Discussion with Joan Brennecke, Caryn Heldt, and Julie Liu

**(123) 3D Printing Keynote (Invited Talks)**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 333

Nima Yazdanpanah, Chair  
Lin Li, Co-Chair

**Sponsored by:** 3D Printing

**12:30** Introductory Remarks

**12:35 Paper 123a:** Nano- and Microfabricated Hydrogels for Regenerative Engineering — *Ali Khademhosseini*

**1:05 Paper 123b:** Commercial Scale Manufacturing of a Pharmaceutical Product Using Powder-Liquid 3D Printing Technology — *Timothy Tracy*

**1:35 Paper 123c:** Closing the Circle on Design, Hardware, and Materials for Additive Manufacturing — *Nathan Wilmot*

**2:05 Paper 123d:** Additive Manufacturing and Architected Materials — *Christopher Spadaccini*

**2:35** Panel Discussion

**(124) Advanced Problem Solving in the Chemical Industry I**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 407

Zdravko Stefanov, Chair  
Andrew P. Santos, Co-Chair  
Dana A. Livingston, Co-Chair  
Paul Chauvel, Jr., Co-Chair  
Eldad Herceg, Co-Chair  
Adrian Howe, Co-Chair

**Sponsored by:** Young Professionals Committee (YPC)

**(125) Advances in Algal Biorefineries I**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 315

Sridhar Viamajala, Chair  
Robert Gardner, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**12:30 Paper 125a:** A Multi-Objective Approach for the Integrated Design of Flexible Algae Biorefineries — *Melina Psycha, Antonis C. Kokossis*

**12:55 Paper 125b:** Biodiversity Enhances Multifunctionality in a Life Cycle Assessment of Microalgal Biofuel Production — *David N. Carruthers, Casey M. Godwin, David C. Hietala, Bradley J. Cardinale, Xiaoxia (Nina) Lin, Phillip E. Savage*

**1:20 Paper 125c:** The Effect of High-Intensity Ultrasound on Cell Disruption and Lipid Extraction from Concentrated and Viscous Slurries of *Nannochloropsis* Sp. Biomass — *Shunyu Yao, Srinivas Mettu, Sam Q K Law, Gregory J O Martin, Muthupandian Ashokkumar*

**1:45 Paper 125d:** Borate-Promoted CO<sub>2</sub> Capture for Microalgae Cultivation — *Jayachandra Kolapalli, Agasteswar Vadlamani, Sridhar Viamajala, Sasidhar Varanasi*

**(126) Advances in Machine Learning and Intelligent Systems**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 410

Fani Boukouvala, Chair  
Matthew J. Reaiff, Co-Chair

**Sponsored by:** Data and Information Systems

**12:30 Paper 126a:** On the Value of Global Optimality in Machine Learning Problems: The Case of Feature Selection for Linear Support Vector Machines — *Adam Beitz, Mark Blenner, Joseph Scott*

**12:49 Paper 126b:** Towards Developing a Learning Based Evolutionary Assistive Paradigm for Surrogate Selection (LEAPS2) — *Sushant S Garud, Iftekhar A. Karimi, Markus Kraft*

**1:08 Paper 126c:** Explore the Potential of Machine Learning in Building Reaction Models for Chemical Industry — *Bo Shuang, Anil Mehta, Kenric Marshall, Tong Zhang, Nikolaos V. Sahinidis*

**1:27 Paper 126d:** Data-Driven Optimization with Implicit Constraints: Application to an Ethane Steam Cracking Process — *Burcu Beykal, Melis Onel, Onur Onel, Efstratios N. Pistikopoulos*

**1:46 Paper 126e:** Recurrent Neural Networks, Numerical Integrators and Nonlinear System Identification — *Tom S. Bertalan, Rob Farber, Thomas Thiem, Felix Dietrich, Ioannis G. Kevrekidis*



**2:05 Paper 126f:** Data-Driven Identification of Interpretable Reduced-Order Models Using Sparse Regression — **Abhinav Narasingam, Joseph Sangil Kwon**

**2:24 Paper 126g:** A Comparison of Mathematical Optimization and Deep Reinforcement Learning for Supply Chain Materials Planning — **Christian D. Hubbs, Satyajith Amaran, John M. Wassick, Nick Sahinidis, Ignacio E. Grossmann**

**2:43 Paper 126h:** Dimensional Analysis Based Uncertainty Quantification: Modeling of Erosion in Pipeline Transportation — **Wei Dai, Selen Cremaschi**

**(127) Advances in Protein Expression, Post-Translational Modification and Biomanufacturing**  
**Monday, Oct 29, 12:30 PM**  
Westin Convention Center, Westmoreland East

Bradley C. Bundy, Chair  
Tamara L. Kinzer-Ursem, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 127a:** Transient Recombinant Protein Production in Glycoengineered Plant Cell Suspension Cultures for Rapid Response Applications — **Sara C. Sukenik, Kalimuthu Karuppanan, Qiongyu Li, Carlito B. Lebrilla, Somen Nandi, Karen A. McDonald**

**12:48 Paper 127b:** Accelerated Virus-Less Generation of Stable Insect Sf9 Cell Lines for High-Yield Production of Influenza Vaccines — **Christine Yee, Prabhu Ponnandy, Andrew Zak, Fei Wen**

**1:06 Paper 127c:** Hyper Extracellular Production of Single-Chain Variable Fragments (scFvs) Using Recombinant *E. coli* By Fed-Batch Culture Based on Do-Stat — **Jun-ichi Horiuchi, Yoichi Kumada, Yuichiro Sakamoto**

**1:24 Paper 127d:** A Simple and Scalable Hydrogel-Based 3D System for Culturing Protein-Producing Cells — **Qiang Li, Haishuang Lin, Ou Wang, Yuguo Lei**

**1:42 Paper 127e:** A Synthetic Biology Platform for Flexible and on-Demand Drug Manufacturing — **Jicong Cao, Pablo Perez-Pinera, Timothy K. Lu**

**2:00 Paper 127f:** Analyzing ER Stress and UPR Activation in Highly Producing Chinese Hamster Ovary (CHO) Cell Lines — **Dyllan Rives, Sarah W. Harcum, Mark Blenner**

**2:18 Paper 127g:** Production of Functional Protein Materials Via Recombinant Expression and Self-Assembly — **Julie A. Champion**

**(128) Area Plenary: Adsorption and Ion Exchange I - In Honor of Peter Monson I (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 301

Stefano Brandani, Chair  
Peter I. Ravikovitch, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**12:30 Paper 128a:** On the Flexibility of Porous Materials — **Lev Sarkisov**

**12:55 Paper 128b:** MOF and Zeolite Membranes and Catalysts — **Michael Tsapatsis**

**1:15 Paper 128c:** Size-Independent Separation of Functionalized Nanoparticles on Porous Substrates — **Kolattukudy Santo, Aleksey Vishnyakov, Alexander Neimark**

**1:35 Paper 128d:** Necessity of Nanowindow Concept in Adsorption and Separation Science in Single Atomic Layer Materials — **Fernando Vallejos-Burgos, Katsumi Kaneko**

**1:55 Paper 128e:** Multi-Scale Modelling of the Synthesis of Nanoporous Silica Materials — **Miguel Jorge**

**2:15 Paper 128f:** Advanced Characterization of Nanoporous Materials: Effect of Pore Size and Temperature on the Adsorption and Phase Behavior of Wetting and Nonwetting Fluids — **Matthias Thommes**

**2:35 Paper 128g:** Combined Molecular- and Process-Level Modeling to Evaluate Metal-Organic Frameworks for Post-Combustion CO<sub>2</sub> Capture — **Karson Leperi, Benjamin Bucior, Joseph T. Hupp, Omar K. Farha, Fengqi You, Randall Q. Snurr**

**(129) Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering II (Invited Talks)**  
**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 327

Amy M. Peterson, Chair  
Julie N. L. Albert, Co-Chair

**Sponsored by:** Polymers

**12:30 Paper 129a:** Printing Semiconductor Polymers to Order — **Ying Diao**

**1:05 Paper 129b:** Enhancing the Optical Performance of Polypropylene in Extrusion Blow Molded Applications — **Nathan Mehl**

**1:40 Paper 129c:** Weld Formation in Material Extrusion Additive Manufacturing — **Jonathan Seppala**

**2:15 Paper 129d:** Taking Advantage of Nature's Building Blocks for the Advancement of Bio-Based Polymers and Composites — **Joseph F. Stanzione III**

**(130) Area Plenary: Future Directions in Applied Mathematics and Numerical Analysis (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 409

Ashlee N. Ford Versypt, Chair  
Yash Puranik, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

**12:30 Paper 130a:** Efficient Computation of Local Sensitivity Information for Nonsmooth Process Models — **Kamil A. Khan**

**12:55 Paper 130b:** A Novel Geometric Based Algorithm to Solve Multiparametric Programming Problems — **Justin Katz, Baris Burnak, Efstratios N. Pistikopoulos**

**1:20 Paper 130c:** Bayesian Machine Learning Modeling of a Reformer Furnace Using CFD Data — **Anh Tran, Madeleine Pont, Andres Aguirre, Helen Durand, Marquis Crose, Panagiotis D. Christofides**

**1:45 Paper 130d:** Image-Based Modeling of Fibroblasts Modifying PDGF-BB Gradient Explains Cells' Alternated Directional Decision during Chemotaxis in a Microfluidic Maze — **Long Quang Pham, Lydia N. Rodrigues, Vishnu Deep Chandran, David Chege, Timothy Dijamco, Nhat-Anh N. Tong, Roman Voronov**

**2:10 Paper 130e:** Multiscale Computational Modeling of Renal Interstitial Cross-Talk at the Onset of Diabetic Kidney Disease — **Minu R. Pilvankar, Steve M. Ruggiero, Ashlee D. Bucher, Ashlee N. Ford Versypt**

**2:35 Paper 130f:** Controllability of the Influenza Virus-Host Protein-Protein Interaction Network: Engineering Insights into Host-Virus Interactions — **Emily E. Ackerman, Jason E. Shoemaker**

**(131) Area Plenary: Leaders in Biomaterials (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 328

Eun Ji Chung, Co-Chair  
Adrianne M. Rosales, Co-Chair

**Sponsored by:** Biomaterials

**12:30 Paper 131a:** Fibrous Proteins – Inspiration, Design and Biomaterials — **David L. Kaplan**

**1:20 Paper 131b:** Invited Speaker — **Jennifer H. Elisseeff**

**2:10 Paper 131c:** Controlled Polymer Assemblies to Promote Drug Delivery and Cellular Genome Editing — **Theresa M. Reineke**

**(132) Area Plenary: Sustainable Biorefineries (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 316

Mark Mba Wright, Chair  
Robert C. Brown, Co-Chair  
Peyman Fasahati, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**12:30 Paper 132a:** Towards Carbon-Negative Bioenergy and Bioproduct Systems using Renewable Electricity — **Christopher M. Saffron**

**1:05 Paper 132b:** Perspective on Carbon Utilization for Fuels, Chemicals, and Materials: Case Studies on Thermal and Catalytic Biomass Processing — **Joshua Schaidle**

**1:40 Paper 132c:** Plenary Presentation — **Wenzhen Li**

**(133) Area 8E Plenary: Electronic and Photonic Materials: Industry and Academia (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 330

Aaron T. Fafarman, Chair

**Sponsored by:** Electronics and Photonics

**12:30 Paper 133b:** CdTe Photovoltaics: High Efficiency and Low Cost at Multi-GW Scale — **Bill Huber**

**12:51 Paper 133f:** Solution Phase Synthesis of Inorganic Nanoparticle, Films and Electronic Devices — **Rakesh Agrawal**

**1:12 Paper 133g:** Silicon Nanocrystal Quantum Dots — **Brian A. Korgel**

**1:33 Paper 133e:** Photoluminescence and Photoconductivity: Secret Weapons to Engineer Printable Photovoltaics Based on CZTS, ClGS, and Hybrid Perovskites — **Hugh W. Hillhouse**

**1:54 Paper 133d:** Making Smart Windows Smarter — **Yueh-Lin Loo**

**2:15 Paper 133c:** Alta Devices: Empowering Autonomy — **Claudio Canizares**

**2:36 Paper 133a:** Industrial Applications of Basic Science: From Photovoltaics to Quantum Computing — **Richard Haight**

### (134) Biosensors, Bodiagnosis and Bioprocess Monitoring: Materials and Devices

**Monday, Oct 29, 12:30 PM**  
Westin Convention Center,  
Westmoreland West-Central

Adam Melvin, Chair  
Kevin J. Cash, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 134a:** An Optical Near Infrared Doxorubicin Sensor Discovered By Spectroscopic and Chemometric Analysis of Nanosensor Libraries — **Jackson Travis Del Bonis-O'Donnell, Rebecca Pinals, Sanghwa Jeong, Ami Thakrar, Russ Wolfinger, Markita Landry**

**12:48 Paper 134b:** Toehold-Mediated DNA Strand Displacement Reactions for Quantitative Paper-Based Diagnostics — **Elizabeth Phillips, Taylor Moehling, Jacqueline Linnes**

**1:06 Paper 134c:** Integration of Surface-Enhanced Raman Scattering and Dielectrophoresis for Rapid Separation and Detection of Bacteria in Real-Time — **Qiuming Yu, Daniel David Galvan**

**1:24 Paper 134d:** Non-Invasive Plasmonic Biosensors for in Situ Glucose Monitoring — **Nihan Yonet-Tanyeri, Ji Eun Park, Richard P. Van Duyn, Milan Mrksich**

**1:42 Paper 134e:** Effects of Low Dose Ionizing Radiation on Microorganisms for Creating Inconspicuous Biosentinels — **Molly Wintenberg, Lisa Manglass, Nicole Martinez, Mark Blenner**

**2:00 Paper 134f:** Bio-Conjugated, Single-Use Biosensor for the Detection of Biomarkers of Prostate Cancer — **Yifan Dai, Jiwei Yao, Yuan Wang, Chung-Chiun Liu**

**2:18 Paper 134g:** Sedimentation Separation of Red Blood Cells and Bacteria for Rapid Diagnosis of Blood Infections — **William G. Pitt, Mahsa Alizadeh, Ryan L. Wood, Alex K. Hunter, Rebekah N. Torgesen**

**2:36 Paper 134h:** Integrated Point of Care Device for Nucleic Acid Extraction, Isothermal Amplification, and Fluorescence-Based on-Line Detection of Viral Genetic Material — **Jackelin Mendoza-Ramos, Everardo González-González, Andres Gracia-Rubio, Grissel Trujillo-de Santiago, Mario Moisés Alvarez, Sergio Omar Martínez-Chapa**

### (135) Carbon Nanomaterials Graduate Student Award Session

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center,  
311

Anju Gupta, Chair  
Markita Landry, Co-Chair  
Anson Ma, Co-Chair

**Sponsored by:** Carbon Nanomaterials

**12:30 Paper 135a:** Application of Novel Porous Graphene Nanoplatelets Composites for Enhanced Heat Transfer Properties — **Aniket Rishi, Satish Kandlikar, Anju Gupta**

**12:45 Paper 135b:** 1-Dimensional Carbon Nanoparticles for Functional Biomolecule Delivery to Mature Plants — **Gozde Sultan Demirel, Huan Zhang, Juliana Matos, Roger Chang, Linda Chio, Brian Staskawicz, Markita Landry**

**1:00 Paper 135c:** Electricity from Asymmetric Chemical Doping of Single-Walled Carbon Nanotubes — **Albert Tianxiang Liu, Yuichiro Kunai, Anton Cottrill, Michael Strano**

**1:15 Paper 135d:** Graphene Oxide Nanocomposite Hydrogels Capable of Wastewater Dye Sequestration — **Elisa A. Torrico Guzmán, Stephen Kennedy, Samantha A. Meenach**

**1:30 Paper 135e:** Addressing the Isomer Cataloging Problem for Nanopores in Graphene and Other 2D Materials — **Ananth Govind Rajan, Kevin Silmore, Jacob Swett, Daniel Blankschtein, Michael Strano**

### (136) CAST Director's Student Presentation Award Finalists

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center,  
408

Ruth Misener, Chair  
Dimitrios V. Papavassiliou, Co-Chair

**Sponsored by:** Computing Systems and Technology Division

**12:30 Paper 136a:** Novel Approaches for the Integration of Supply Chain Planning and Scheduling — **Braulio Brunaud, Satyajith Amaran, Scott J. Bury, John M. Wassick, Ignacio E. Grossmann**

**12:49 Paper 136b:** Optimal Demand Response Operation of an Industrial Air Separation Unit Using Data-Driven, Scheduling-Relevant Dynamic Models — **Calvin Tsay, Michael Baldea, Jun Shi, Ankur Kumar, Jesus Flores-Cerrillo**

**1:08 Paper 136c:** Integration of Planning, Scheduling and Control Using Feasibility Analysis and Surrogate Models — **Lisia S Dias, Marianthi Ierapetritou**

**1:27 Paper 136d:** Decode: Detection of Communities for Optimization Decomposition — **Andrew Allman, Wentao Tang, Prodromos Daoutidis**

**1:46 Paper 136e:** Identification of Optimal Dopant Patterns in a Doped Perovskite Oxygen Carrier — **Christopher L. Hanselman, Dominic Alfonso, Jonathan W. Lekse, De Nyago Tafen, Christopher Matraga, David C. Miller, Chrysanthos E. Gounaris**

**2:05 Paper 136f:** Unipopt: Univariate Projection-Based Optimization without Derivatives — **Ishan Bajaj, M. M. Faruque Hasan**

**2:24 Paper 136g:** Hierarchical MPC Schemes for Periodic Systems Using Stochastic Programming Techniques — **Ranjeet Kumar, Victor M. Zavala**

**2:43 Paper 136h:** Concurrent Canonical Variate Analysis for Process Operating Condition Deviations and Dynamic Anomalies Monitoring — **Weike Sun, Benben Jiang, Richard D. Braatz**

### (137) Cellulose Based Materials II

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center,  
325

Sudhagar Mani, Chair  
Joseph F. Stanzione III, Co-Chair

**Sponsored by:** Forest and Plant Bioproducts Division

**12:30 Paper 137a:** Towards Economical and Sustainable Production of Wood Based Nanomaterials — **J. Y. Zhu**

**12:55 Paper 137b:** High Shear Capillary Rheometry of Cellulose Nanomaterials for Industrial Relevant Processing — **Bradley Sutliff, Jeffrey Youngblood, Michael J. Bortner**

**1:20 Paper 137c:** Towards Standardization of Laboratory Preparation Procedure for Uniform Cellulose Nanopapers — **Maresh Parit, Burak Aksoy, Zhijia Jiang**

**1:45 Paper 137d:** Emerging Cellulose Nanocrystals for Threshold Scale Inhibition: A Step Forward in Universal Biomass-Based Crystal Engineering — **Amir Sheikhi, Ashok Kakkar, Theo G. M. van de Ven**

### (138) Colloidal Hydrodynamics: Structure and Microrheology

**Monday, Oct 29, 12:30 PM**  
Omni William Penn Hotel, Frick

Roseanna N. Zia, Chair  
Lilian Hsiao, Co-Chair

**Sponsored by:** Fluid Mechanics

**12:30 Paper 138a:** Microstructural Evolution of Dilute Colloidal Gels during Shear Startup — **Bharath Rajaram, Farzaneh Taslimi, Ali Mohraz**

**1:00 Paper 138b:** Microstructure and Rheology of Associative Soft Particles Glasses — **Fardin Khabaz, Maddalena Mattiello, Michel Cloitre, Roger T. Bonnecaze**

**1:15 Paper 138c:** The Hydrodynamics of the Colloidal Glass Transition — **Roseanna N. Zia, Jialun Wang, Gregory B. McKenna, Xiaoguang Peng, Xi Li**

**1:30 Paper 138d:** Controlling Dynamic Structures in Linked Colloidal Particle Chains — **Steve Kuei, Sibani Lisa Biswal**

**1:45 Paper 138e:** Dynamic Evolution of the Internal Structure of a Drying Colloid-Polymer Film — **James F. Gilchrist, Thitiporn Kaewpetch**

**2:00 Paper 138f:** From Hindered to Promoted Settling in Dispersions of Attractive Colloids — **James Swan, Andrew Fiore**

**2:15 Paper 138g:** *In Situ* Nanostructure Characterization of Complex Fluids Under Arbitrary Processing Flows — **Patrick Corona, L. Gary Leal, Matthew E. Helgeson**

**2:30 Paper 138h:** Diffusion and Equilibrium Structure of Bi-Disperse Colloidal Suspensions Confined By a Spherical Cavity — **Emma Gonzalez, Christian Aponte-Rivera, Roseanna N. Zia**

**2:45 Paper 138i:** Oscillatory Active Nanorheology Simulations of Colloidal Suspensions: Effect of Probe Size — **Dinesh Sundaravadivelu Devarajan, Rajesh Khare**



**(139) Computational Solid State Pharmaceutics****Monday, Oct 29, 12:30 PM**

Westin Convention Center, Washington

Yuri Abramov, Chair  
Athanas Koynov, Co-Chair**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum**12:30 Paper 139a:** Rapid Temperature Correction to Lattice Energy Landscape for Crystal Structure Prediction— *Mingjun Yang\**, *Eric Dybeck\**, *Guangxu Sun*, *Geoffrey Wood*, *Virginia Burger*, *Yang Liu*, *Peiyu Zhang*, *Jian Ma*, *Alan Jiang*, *Bruno C. Hancock*, *Shuhao Wen***12:55 Paper 139b:** Understanding the Effect of Changing Complexities of Potential Energy Functions on the Entropic Contribution to Free Energy Differences of Organic Polymorphs — *Nathan Abraham*, *Michael Shirts*, *Eric Dybeck\**, *Natalie Schieber***1:20 Paper 139c:** Improved Efficiency in the *Ab Initio* Generation of Crystal Structures — *Isaac Sugden*, *Claire S. Adjiman*, *Constantinos C. Pantelides***1:45 Paper 139d:** Molecular Crystal Structure Prediction with Gator and Genarris — *Noa Marom***2:10 Paper 139e:** Combining Simulation and Experiment to Understand Polymorph Selection of Drug Molecules in Different Solvents — *Chengxiang Liu*, *Geoffrey Wood*, *Samir Kulkarni*, *Erik E. Santiso***2:35 Paper 139f:** Novel Computational Approaches to Support Pharmaceutical Solid State Chemistry Tasks — *Yuri Abramov***(140) Data Analytics for Process Prediction****Tuesday, Oct 30, 12:30 PM**

Westin Convention Center, Fayette

Shekhar Viswanath, Chair  
Jacob Albrecht, Co-Chair**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum**12:30 Paper 140a:** A Reaction Database for Small Molecule Pharmaceutical Processes Integrated with Process Information: Future Developments — *Emmanouil Papadakis*, *Anjan Kumar Tula*, *Rafiqul Gani***12:55 Paper 140b:** Learning to Design and Validate Small-Molecule Synthetic Routes from Historical Reaction Data — *Connor W. Coley*, *Pieter Plehiers*, *Wengong Jin*, *Hanyu Gao*, *Regina Barzilay*, *Tommi S. Jaakkola*, *William H. Green*, *Klavs F. Jensen***1:20 Paper 140c:** Using Machine Learning to Recommend Reaction Conditions and Quantifying Similarity of Catalysts, Solvents, and Reagents — *Hanyu Gao*, *Thomas Struble*, *Connor W. Coley*, *William H. Green*, *Klavs F. Jensen***1:45 Paper 140d:** Applying Data Science Techniques to Solubility Data for Synthetic Compounds: An Expedited End-to-End Workflow from Data Collection to Crystallization Process Design — *Michael Lovette*, *Seth Huggins***2:10 Paper 140e:** Optimizing Drying Profile of Polymeric Drug Products Using Machine Learning and First Principle Modeling — *Rishi Mehan*, *SVB Janardhan Garikipati*, *RaviChandra Palaparthi***2:35 Paper 140f:** Leveraging Deep Learning for Pharmaceutical Discovery Lead Profiling — *Jacob Albrecht*, *Marcello Riccottoni*, *Wilson Shou*, *Stephen Johnson***(141) Data Analytics in Operational Support****Monday, Oct 29, 12:30 PM**

Westin Convention Center, Fayette

Shekhar Viswanath, Chair  
Jacob Albrecht, Co-Chair**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum**12:30 Paper 141a:** Prediction of Risk in Drug Substance Starting Material Selection — *Brandon Reizman*, *Justin Burt*, *Scott Frank*, *Salvador Garcia-Muñoz***12:55 Paper 141b:** An Intelligent Machine for Document Preparation — *Shekhar Viswanath*, *Jared Fennell*, *Matthew Yates*, *Justin Burt*, *Jason Yazell*, *Rachel Kuhr*, *Brad Strum*, *Prafulla Krishna*, *Kalpesh Barar*, *Rucha Kulkarni*, *Harshad Kulkarni***1:20 Paper 141c:** Data-Driven Real-Time Operation Support for Decontamination Processes in Biopharmaceutical Drug Product Manufacturing — *Anicia Zeberli*, *Sara Badr*, *Christian Siegmund*, *Markus Mattern*, *Hirokazu Sugiyama***1:45 Paper 141d:** Ontology-Driven Models and Algorithms for Pharmaceutical R&D Activity Planning — *Nikolaos Lappas*, *Michael Semo*, *Scott Frank*, *Shekhar Viswanath*, *Justin Burt*, *Shankararaman Vaidyaraman*, *Chrysanthos E. Gounaris***2:10 Paper 141e:** Development of an End-to-End Data Management and Visualization System for Cell Culture Process Development — *Brian Doyle*, *Delyan Rusev*, *Itze Lamadrid*, *Winnie Yeung*, *Gayle E. Derfus*, *Yunling Bai*, *Cary F. Opel***2:35 Paper 141f:** Holmes: An Ontology-Based Knowledge Management System for Pharmaceutical Engineering — *Miguel Francisco Remolona*, *Venkat Venkatasubramanian***(142) Developments in Petroleum and Biofuels Refining Technologies****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 323

Paul M. Mathias, Chair  
Robert Sigal, Co-Chair**Sponsored by:** Fuels and Petrochemicals Division**12:30 Paper 142a:** Methaforming Produces Gasoline from Naphtha and Methanol at 1/3 the Current Cost — *Stephen Sims***12:51 Paper 142b:** Oxidative Desulphurisation Using Vortex Based Hydrodynamic Cavitation with Water Dispersed in Organic Phase — *Peter Delaney***1:12 Paper 142c:** Low Pressure Hydrodeoxygenation of Liquid Phase Pyrolysis Oil and Refinery Intermediates — *Klara Treusch*, *Nikolaus Schwaiger*, *Anna Huber*, *Thomas Pichler*, *Matthaeus Siebenhofer*, *Peter Pucher***1:33 Paper 142d:** Plausible Pathway to Meet IMO 2020 Global Sulfur Cap — *Amaka Waturuocha*, *Glixon Mavarez Nava*, *Michael Volk*, *Dwijen Banerjee***1:54 Paper 142e:** Modification of FCC Slurry Oil Used for Producing High-Grade Paving Asphalt — *Lingrui Cui*, *Fahai Cao*, *Mannian Ren***2:15 Paper 142f:** Spherical Polymer Brushes Bearing Pyrrolidone Groups As Novel Nickel Remover for Crude Oil — *Tong Geng*, *Jun Xu*, *Mannian Ren*, *Fahai Cao***(143) Dynamics and Modeling of Particulate Systems: Discrete and Continuum****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 414

M. Silvina Tomassone, Chair  
Jorg Theuerkauf, Co-Chair**Sponsored by:** Solids Flow, Handling and Processing**12:30 Paper 143a:** A DEM Study of Shear Flows of a Binary Mixture of Non-Spherical Particles — *Jiecheng Yang*, *Yu Guo*, *Jennifer S. Curtis***12:48 Paper 143b:** Comparisons of Continuum FEM Models of Hopper Flow of Particulate Materials to Experimental Measurements — *Kunal S. Pardikar*, *Carl R. Wassgren*, *Tyler L. Westover***1:06 Paper 143c:** Development of a Coupled CFD – DEM Simulation Method for a Tablet Coating Process — *Peter Böhling*, *Wen-Kai Hsiao*, *Frederik Detobel*, *James Holman*, *Matthew Metzger*, *Laura Wareham*, *Johannes G. Khinast***1:24 Paper 143d:** Implementation of a Non-Local Granular Fluidity Model in Openfoam for Simulation in Arbitrary 3D Geometries — *Jonathan J. Stickel*, *Hariswaran Sitaraman*, *James J. Lischkes*, *Mohammad Rahimi***1:42 Paper 143e:** Multi-Scale Modelling of Biomass Gasification: The Effects of Intraparticle Transfer on Syngas and Biochar Production — *Zhiyi Yao*, *Avi Uzi*, *Tiansu Ge*, *Chi-Hwa Wang***2:00 Paper 143f:** Coarse-Grained Discrete Element Model for Powder Shear Flow — *Hideya Nakamura*, *Hiroharu Takimoto*, *Shuji Ohsaki*, *Satoru Watano***2:18 Paper 143g:** Numerical and Experimental Studies of Granular Materials in the Quasi-Static Regime — *Lyes Ait Ali Yahia*, *Riccardo Maione*, *Ali Ozel*, *Raffaella Ocone***(144) Efficient Processing of Lignin to Bioproducts and Biofuels I****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 318

Bin Yang, Chair  
Arthur J. Ragauskas, Co-Chair  
Joshua Yuan, Co-Chair  
Ning Sun, Co-Chair**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**12:30 Paper 144a:** Solid-State Depolymerization and Isolation of Lignin from Lignocellulosic Biomass — *Ning Li, Yanding Li, Chang Geun Yoo, Xiaohui Yang, Xuliang Lin, John Ralph, Xuejun Pan*

**12:45 Paper 144b:** Catalytic Depolymerization and Liquefaction of Lignin in Ionic Liquid By  $\text{SO}_4^{2-}/\text{ZrO}_2$  in a Flow through System — *Wang Xiuhui, Qian Eika W*

**1:00 Paper 144c:** The Impact of Acid Site Concentration and Pore Diameter on the Cracking of Lignin Derived Monomers in Zeolites — *Michael Stellato, Carsten Sievers, Andreas S. Bommarius*

**1:15 Paper 144d:** High Energy Density Fuels Produced from Lignin-Derived Intermediates and Refinery Waste Gas Streams — *Maoqi Feng, Bin Yang*

**1:30 Paper 144e:** Towards Valorization of Biorefinery Waste to Polyhydroxyalkanoate: Structural Characterization and Mechanisms — *Naijia Hao, Somnath Shinde, Zhihua Liu, Joshua Yuan, Arthur J. Ragauskas*

**1:45 Paper 144f:** Characterization of Deep Eutectic Solvent Extracted Lignin Streams from Endocarp Biomass — *Wenqi Li, Kirtley Amos, Mi Li, Yunqiao Pu, Arthur J. Ragauskas, Seth Debolt, Yang-Tse Cheng, Jian Shi*

**2:00 Paper 144g:** Muconic Acid Production from an Engineered *Rhodococcus Opacus* — *Zhaoxian Xu, Mingjie Jin*

**2:15 Paper 144h:** Reactivity-Based Fractionation of Lignins Via Reversible Conjunction to Polymeric Amines — *Zhengjun "Glen" Li*

**2:30 Paper 144i:** Understanding and Modeling Effects of Nitrogen Source on Biosynthesis of Polyhydroxyalkanoates from Benzoate By *Pseudomonas Putida* KT2440 — *Zhangyang Xu, Bin Yang*

#### **(145) Electrocatalysis and Photoelectrocatalysis II: Reactors and Processes for CO<sub>2</sub> Reduction** **Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 401

Tae-Sik Oh, Chair  
Meenesh R. Singh, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 145a:** Electrochemical CO<sub>2</sub> Conversion to Valuable Chemicals — *Feng Jiao*

**12:51 Paper 83h:** Development of Devices and Selective Catalysts for the Solar-Driven Reduction of CO<sub>2</sub> to fuels — *Marcel Schreier, Michael Grätzel, Yogesh Surendranath*

**1:12 Paper 145c:** Bimetallic Nanoporous Pd Alloys as CO Tolerant Electrocatalysts for the Electrohydrogenation of CO<sub>2</sub> to Formate — *Swarnendu Chatterjee, Yawei Li, Joshua Snyder*

**1:33 Paper 145d:** Electrochemical Promotion of Catalysis: Non-Faradaic Effects of Applied Potential on CO<sub>2</sub> Hydrogenation and Ethylene Oxidation Reactions — *Mark Sullivan, Dimitris Zagoraios, Constantinos Vayenas, Yuriy Román-Leshkov*

**1:54 Paper 145e:** Nano- to Macro Scale Morphological Impacts on CO<sub>2</sub> electroreduction Product Selectivity over Cu Catalysts — *Samaneh Sharifi Golru, Alexandros N. Karaiskakis, Elizabeth J. Biddinger*

**2:15 Paper 145f:** Insights into the Electrocatalytic Conversion of CO<sub>2</sub> into CO, Ethylene, and Ethanol in Alkaline Media — *Paul J. A. Kenis, Andrew A. Gewirth*

**2:36 Paper 145g:** Insights on the Electrochemical Reduction of Carbon Dioxide Using Solid Oxide Electrolysis Cells — *Juliana S. A. Carneiro, Xiang-Kui Gu, Eranda Nikolla*

#### **(146) Energy & the Environment U.G. Research Session (Invited Talks)**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 302

Cory Thomas, Chair

**Sponsored by:** Young Professionals Committee (YPC)

**12:30 Paper 146b:** Understanding the impact of compression on the performance of Thin Flexible Fuel Cell (TFFC) — *Matthew Mayer*

**12:55 Paper 146c:** Characterizing microplastic degradation: Traditional and novel techniques for analyzing plastics and their degradation compounds in simulated marine environments — *Xiaoxiao Wang*

**1:20 Paper 146d:** Utilizing Microalgae to Remove Phosphorus from Wastewater Effluent Streams through Hydrothermal Liquefaction — *Amanda C. Ruhmann*

**1:45 Paper 146e:** Title Pending — *Guilherme de Oliveira*

**2:10 Paper 146f:** Title Pending — *Ridhish Kumar*

#### **(147) Engineering Geologic Carbon Dioxide Storage Systems**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 321

Kanwal Mahajan, Chair  
Rameshwar D. Srivastava, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**12:30 Paper 147a:** An Overview of Recent Efforts Under the Department of Energy's Carbon Storage Program: Moving CCS Towards Commercialization — *Mary Sullivan, Erik Albenze, Kanwal Mahajan, Traci Rodosta*

**12:52 Paper 147b:** Planning the First South African Pilot CO<sub>2</sub> Storage Project — *Mackenzie Scharenberg, Neeraj Gupta, Charlotte Sullivan, Michael Heinrichs, Andrew Burchwell*

**1:14 Paper 147c:** Chemical Impacts of CO<sub>2</sub> Intrusion into Heterogeneous Caprock — *Ting Xiao, Brian McPherson, Nathan Moodie, Trevor Irons, Wei Jia, Richard Esser*

**1:36 Paper 147d:** Implementing and Validating Active Reservoir and Brine Management Strategies for the Enhancement of the Geologic Storage of Carbon Dioxide: An Update — *David Nakles, John A. Hamling, Ryan J. Klapperich*

**1:58 Paper 147e:** Evolution of Transport and Mechanical Properties of Mt Simon Sandstones Due to Interaction with Brine/CO<sub>2</sub> — *Zhuofan Shi, Lin Sun, Kristian Jessen, Theodore Tsotsis*

**2:20 Paper 147f:** Optimization of CO<sub>2</sub>-Enhanced Oil Recovery with CO<sub>2</sub> Storage in a Mature Oil Field — *William Ampomah, Robert Balch, Robert Will, Reid Grigg, Martha Cather*

**2:42 Paper 147g:** How Much Oil and CO<sub>2</sub>? at What Cost? Bounding the Quantities of Produced Oil and Stored CO<sub>2</sub> from CO<sub>2</sub> EOR in Conventional Oil Fields in the United States — *David Morgan, Donald Remson, Tim Grant*

#### **(148) Environmental Division Awards and Honors (Invited Talks)**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 319

Leslie M. Shor, Chair  
Debalina Sengupta, Co-Chair  
Nga Lee Ng, Co-Chair

**Sponsored by:** Environmental Division

#### **(149) Experiences in Teaching Process Safety**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 335

Kenneth R. Cox, Chair  
Tracy Carter, Co-Chair  
Benjamin John Davis, Co-Chair

**Sponsored by:** Product Design

**12:30 Paper 149a:** Using Team Building to Focus the Intersection of Diversity and Inclusion with Process Safety Practice — *Tom Spicer III*

**12:55 Paper 149b:** Developing a Mindset of Safety in Students — *Sharon G. Sauer, Adam J. Nolte*

**1:20 Paper 149c:** Process Safety Instructional Enhancements Implemented in a Two-Semester Chemical Process Design Course — *Matthew L. Alexander*

**1:45 Paper 149d:** Integration of Process Safety Experience in Research Project into Undergraduate Process Design Courses — *Andrew Tong, Mandar Kathe, Liang-Shih Fan, Jeffrey J. Chalmers, David L. Tomasko*

**2:10 Paper 149e:** Integrating Chemical Process Safety across the Curriculum — *Tracy Carter*

**2:35 Paper 149f:** Where Does Process Safety Fit into the Chemical Engineering Curriculum? — *Kenneth R. Cox*

#### **(150) Experimental Investigation of Fluidization Processes**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 415

Clay Sutton, Chair  
Ben Freireich, Co-Chair

**Sponsored by:** Fluidization and Fluid-Particle Systems

**12:30 Paper 150a:** Experimental Observation of the Initial Stages of Localized Fluidization — *Sarah E. Mena, Florian Brunier, Jennifer S. Curtis, Pierre Philippe*

**12:48 Paper 150b:** Bubbles Distribution in a 0.6-m-Diameter Disk and Donut Fluidized Bed Stripper — *Allan Issangya, S. B. Reddy Karri, T. M. Knowlton, Ray Cocco, Ben Freireich*

**1:06 Paper 150c:** Magnetic Resonance Imaging of Injected Bubble and Jet Dynamics in Fluidized Beds — *Christopher M. Boyce, Alexander Penn, Maxim Lehnert, Klaas P. Pruessmann, Christoph R. Müller*

**1:24 Paper 150d:** Experimental Validation of Indirect Conduction Model and Biot Number Analysis for Wall-to-Particle Heat Transfer — *Ipsita Mishra, Aaron Lattanzi, Aaron Morris, Christine M. Hrenya*

**1:42 Paper 150e:** Heat Transfer Measurement and Modelling in a Fluidized Bed with Pulsed Gas Flow — *Dening Jia, Xiaotao Bi, C. Jim Lim, Shahab Sokhansanj, Atsushi Tsutsumi*

**2:00 Paper 150f:** Behavior of Nanosized TiO<sub>2</sub> Catalyst in a Microjet and Vibration Assisted Fluidized Bed — *Keju An, Jean M. Andino*

**2:18 Paper 150g:** Identification and Characterization of Meso-Scale Flow Structure in the Dense Gas-Solid Flow in a Fluidized Bed — *LI Niu, Mengxi Liu, Zhimin Chu*

**2:36 Paper 150h:** Kutta-Joukowski Force: The Radial Distribution of Particles Concentration in a Riser — *Yiping Fan, Chen Li, Mengxi Liu, Chunxi Lu*

**(151) FEW Nexus Topical Plenary: Engineering More Sustainable Primary Production (Invited Talks)**  
**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 317

Leslie M. Shor, Chair  
Fengqi You, Co-Chair

**Sponsored by:** The Food-Energy-Water Nexus

**12:30 Paper 151a:** Water Dynamics in Plants and the Innovations for Agriculture They Inspired — *Abraham D. Stroock*

**1:20 Paper 151b:** Electrochemical Conversion of Ammonia and Nitrogen for Sustainable Food-Energy-Water — *Gerardine G. Botte*

**2:10 Paper 151c:** Encapsulation and Nanoparticle Formation for “Non-Standard” Applications — *Robert K. Prud’homme, Rodney D. Priestley, Leslie M. Shor, Douglas Scott, Jie Feng*

**(152) Flow Assurance and Asset Integrity**

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 305

Vikram Subramani, Chair

**Sponsored by:** Upstream Engineering and Flow Assurance Forum

**12:30 Paper 152a:** The Current State of the Knowledge: Wax Deposition Modeling and Up Scaling Challenges — *Nagu Daraboina, Cem Sarica*

**12:50 Paper 152b:** CFD Modeling of Mixed Flow Regime for Gas-Liquid Flows in Vertical Pipe — *Mohammad A. Elyyan, Sravan Kumar Nallamothu, Madhusuden Agrawal*

**1:10 Paper 152c:** The Influence of Surfactants and Nanoparticles on Hydrate Formation in Water-in-Oil Emulsions — *Ashwin Kumar Yegya Raman, Clint P. Aichele*

**1:30 Paper 152d:** Prospects of Amino Acids and Ionic Liquids As a Potential Gas Hydrate Inhibitors for Offshore Flow Assurance — *M. Fahed Qureshi, Tausif Altamash, Majeda Khraisheh, M.a Saleh*

**1:50 Break**

**2:00 Paper 152e:** Flow Assurance Studies with Multiphase Flowloop: High Viscosity Carrier Fluids and Viscous Heating in Hydrate Transporting Systems — *Ben Bbosa, Michael Volk*

**2:20 Paper 152f:** Iron Sulfide Scale Removal from Production Wells By New Chemical Formulation: A Field Application in a Sandstone Reservoir in Egypt — *Emad Hamdy Riad Sr.*

**2:40 Paper 152g:** Modeling Aqueous CO<sub>2</sub> Corrosion in Oil/Water Mixtures — *Kuo Chen Tsai*

**(153) Free Forum on Engineering Education: Junior and Senior Years I**  
**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 411

Elif E. Miskioglu, Chair  
Daniel Knight, Co-Chair

**Sponsored by:** Undergraduate Education

**12:30 Paper 153a:** Integrated Humor in the Engineering Classroom Using Isomorphic Mapping to Improve Learning Outcomes Via Increased Germane Cognitive Load — *Peter J. Ludovice, Jessica Plumley, Wendy Newstetter, David MacNair*

**12:48 Paper 153b:** Making Interactive Simulations and Screencasts More Interactive — *John L. Falconer, Janet deGrazia*

**1:06 Paper 153c:** Advanced Participatory Design – a Tool for Enquiry Based Module Design — *Pavan Inguva, Wenqian Chen, James Campbell, Umang V. Shah, Clemens Brechtelsbauer*

**1:24 Paper 153d:** Introducing Contemporary Topics in a Transport Phenomena Course through Michigan-Themed Projects — *Susan Farhat, Salomon Turgman-Cohen*

**1:42 Paper 153e:** Teaching Energy and Sustainability Using Only Active Learning Pedagogies — *Ian Hosein*

**2:00 Paper 153f:** A Blended Textbook Free Chemical and Biochemical Process Safety Class — *Daniel Forciniti*

**2:18 Paper 153g:** Revealing the Decision-Making Processes of ChE Students in Process Safety Contexts — *Brittany Butler, Emily Dringenberg, Daniel Anastasio, Daniel D. Burkey, Matthew Cooper, Cheryl A. Bodnar*

**(154) Functional Interfaces to Control Pathogenic or Beneficial Microbes**

**Monday, Oct 29, 12:30 PM**  
Westin Convention Center, Pennsylvania East

Katy Kao, Co-Chair  
James Wilking, Co-Chair

**Sponsored by:** Microbes at Biomedical Interfaces

**12:30 Paper 154a:** Biofilm Growth Drives the Selective Targets and Trajectories during the Evolution of Antimicrobial Resistance — *Vaughn Cooper*

**12:55 Paper 154b:** Invited Talk 2: Repeatability of Metabolic Profiles in Multispecies Biofilms – Toward Metrics for Biofilm Comparability — *Nancy J. Lin, Sandra M. Da Silva, Elena Musteata, Yamil Simón-Manso*

**1:20 Paper 154c:** Invited Talk 3: Creating New Separation Processes By Interfacing Engineered Cells with Non-Living Material Interfaces — *Jack Lake, Keith Heyde, Warren Ruder*

**1:45 Break**

**2:00 Paper 154e:** Antifungal Peptide Variants with Reduced Degradation By Fungal Proteases and Improved Antifungal Activity Against Planktonic and Biofilm Cells — *Parisa Moghaddam-Taaheri, Svetlana P. Ikononova, Qin Zeng, Christopher M. Jewell, Amy J. Karlsson*

**2:15 Paper 154f:** Effect of Poly-L-Lysine Molecular Weight on Antibacterial Activity of Polyelectrolyte Multilayer Coated Surfaces — *Dahlia Alkekha, Anita Shukla*

**2:30 Paper 154g:** Antimicrobial Activity of Endogenous Human  $\beta$ -Defensin 3 Produced Via Polyplex Transfection — *Logan Warriner, Daniel W. Pack, David A. Puleo*

**2:45 Paper 154h:** The Impact of Surface Topography on Adhesion and Biofilm Formation of Cyanobacteria — *Suvarna N L. Talluri, Haeyeon Yang, Robb M. Winter, David R. Salem*

**(155) Hydrodynamics of Active Systems**

**Monday, Oct 29, 12:30 PM**  
Omni William Penn Hotel, Phipps

Ubaldo M. Córdova-Figueroa, Chair  
Gwynn Elfring, Co-Chair

**Sponsored by:** Fluid Mechanics

**12:30 Paper 155a:** Active Matter Invasion of a Viscous Fluid and a No-Flow Theorem — *Christopher Miles, Arthur Evans, Michael J. Shelley, Saverio Spagnolie*

**1:00 Paper 155b:** Force Moments of Active Particles — *Babak Nasouri, Gwynn Elfring*

**1:15 Paper 155c:** Dynamics of Active Particles Near a Curved Wall: Guided and Trapped Locomotion — *Pablo Díaz-Hyland, Ubaldo M. Córdova-Figueroa, Nima Sharifi-Mood*

**1:30 Paper 155d:** Phase Behavior of Binary Active Colloidal Systems — *Carlos Silvera Batista, Javier D. Gomez*

**1:45 Break**

**2:00 Paper 155f:** Reduced Viscosity Experienced By Flagella Moving in a Solution of Long Polymer Chains — *Arezoo Ardekani, Yuchen Zhang*

**2:15 Paper 155g:** Simulation of *C. elegans* Swimming in Viscoelastic Fluids via the Immersed Boundary Technique — *Christopher Guido, Jeremy Binagia, Eric S. G. Shaqfeh*

**2:30 Paper 155h:** Active Chromatin Hydrodynamics: Coarse-Grained Modeling and Simulations — *David Saintillan, Michael J. Shelley, Alexandra Zidovska*



**(156) Industrial Applications of Computational Chemistry and Molecular Simulation**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 308

Joseph Golab, Chair  
Martin Sanborn, Co-Chair  
Phillip R. Westmoreland, Co-Chair  
Jonathan Moore, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**12:30 Paper 156a:** Enhanced Coil Dimensions of Polyolefins: Effect of Tacticity and Side Chain Structure — **Mohammad Atif Faiz Afzal, George Rodriguez, Jarod Younker**

**12:50 Paper 156b:** Mechanisms of Halogenated Silane Decomposition on an N-Rich Surface during Atomic Layer Deposition of Silicon Nitride — **Gregory Hartmann, Peter Ventzek, Toshihiko Iwao, Kiyotaka Ishibashi, Gyeong S. Hwang**

**1:10 Paper 156c:** Effect of Lanthanum Doping on Structure, Electronic and Elastic Properties of Perovskite, Pyrochlore Oxide and Lanthanide Titanates: A First Principles Study — **Amar Deep Pathak, Foram Thakkar, Suchismita Sanyal, Hans Geerlings, Arian Nijmeijer**

**1:30 Paper 156d:** Modelling Solubility of Metal Complexes in Non-Aqueous Media from First Principle Calculations: Application to Redox Flow Cell — **Anwesa Karmakar, Ping Yang, Enrique R. Batista**

**1:50 Paper 156e:** Thermophysical, Interfacial and Transport Properties of Low Global Warming Potential Refrigerants from Molecular Theory and Simulations — **Wael A. Fouad, Yuting Li, Lourdes F. Vega**

**2:10 Paper 156f:** Automatic Construction of Collective Variables for Metadynamics Simulations of Drug Permeation through Lipid Membranes — **Fikret Aydin, Jessica M. J. Swanson, Gregory A. Voth**

**2:30 Paper 156g:** Prediction of the Reactivity of Chemical Compounds with Ozone in Water — **Chikashi Shinagawa**

**2:50** Discussion of Industrial Applications.

**(157) In Honor of Doraiswami Ramkrishna's 80th Birthday II (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

Westin Convention Center, Somersset

Jamey D. Young, Chair  
Meenesh R. Singh, Co-Chair

**Sponsored by:** Food, Pharmaceutical & Bioengineering Division

**12:30 Paper 157a:** Protein Diffusion, Convection and Vesicular Transport in the Intestinal Wall: How Ramkrishna's Teachings Helped the Drug Delivery Field — **Nicholas A. Peppas**

**12:55 Paper 157b:** Bio-Oil Upgrading Using Methane: A Mechanistic Study of Model Compound Guaiacol Reactions over Pt-Bi Bimetallic Catalysts — **Arvind Varma, Yang Xiao**

**1:20 Paper 157g:** Mixed Cultures: an Example of Ramki's Enduring Legacies — **Gregory Stephanopoulos**

**1:45 Paper 157d:** The Weighted Ellipsoidal Metric Space (WEMS) Theorem and Stokes Flow Past an Ellipsoid in a Polynomial Ambient Field — **Curtis Martin, Shiyang Wang, Sangtae Kim**

**2:10 Paper 157e:** Integral-Spectral Methods with Healthcare Applications: Cancerous Tumor Treatment, Hemodialysis, and Kidney Malfunction—Some Exciting Opportunities — **Pedro E. Arce, A. Nastasia Allred, Yung-Way Liu, J. Robby Sanders**

**2:35 Paper 157f:** Direct Numerical Simulation of Turbulent Channel Flow and Flow Past Sphere over a Wide Range of Reynold's Number — **Jyeshtharaj B. Joshi**

**(158) In Honor of Michael Smith's 60th Birthday II (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 405

Jeffrey D. Rimer, Chair  
Phillip Christopher, Co-Chair  
Michael A. Smith, Co-Chair  
Alexander Zoelle, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 158a:** Catalytic C-C Bond Forming Reactions for the Transformation of Biomass to Commodity Chemicals — **Raul F. Lobo**

**12:50 Paper 158b:** Evidence for Tunable Electronic Metal-Support Interactions in Carbon-Supported Palladium Catalysts — **Radhika Rao, Raoul Blume, Kathleen Dreyer, Thomas W. Hansen, David Hibbitts, Robert Schlogl, Jean-Philippe Tessonnier**

**1:10 Paper 158c:** Fabrication of Nano-Structured Catalyst Supports By ALD — **Raymond J. Gorte**

**1:30 Paper 158d:** Template-Mediated Tunability of Pores, Polymorphism, and Function in Nanostructured Materials — **Mark A. Snyder**

**1:50 Paper 158e:** Unconventional Pathways for Unconventional Feedstock: The Importance of Simultaneous Optimization of Catalytically Active Sites and Their Environment — **Lars C. Grabow**

**2:10 Paper 158f:** Leveraging DFT with Machine Learning: Applications in Catalysis — **John R. Kitchin**

**2:30 Paper 158g:** Exploiting Mesoporosity for the Design of Novel Materials — **Jeffrey D. Rimer**

**2:45 Paper 158h:** Lithium Silicates for High Temperature CO<sub>2</sub> Capture — **Michael A. Smith**

**(159) In Honor of Pablo Debenedetti II (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 307

Jeffrey R. Errington, Chair  
Andrew Ferguson, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**12:30 Paper 159a:** Understanding Amyloid Co-Assembly Bycharge-Complementary Peptides — **Carol Hall, Qing Shao, Kong M. Wong, Dillon T. Seroski, Anant K. Paravastu, Gregory A. Hudalla**

**12:50 Paper 159b:** Structure and Dynamics of Active Liquid Crystalline Biopolymers — **Juan J. DePablo, Rui Zhang, Margaret L. Gardel, Nitin Kumar**

**1:10 Paper 159c:** Supercritical Fluids and Spray-Drying: Particles for Pharmaceuticals — **Jean W. Tom**

**1:30 Paper 159d:** How to Hit HIV Where It Hurts — **Arup Chakraborty**

**1:50 Paper 159e:** Predicting Protein Interactions to Enhance Stability and Solubility of Therapeutic Antibodies — **Christopher J. Roberts**

**2:10 Paper 159f:** The Putative Liquid-Liquid Transition Is a Liquid-Liquid Transition in Some Atomistic Models of Water — **Jeremy Palmer**

**2:30 Paper 159g:** Water-Mediated Interactions Involving Heterogeneous Molecules, Surfaces, and Phases — **M. Scott Shell**

**(160) In Honor of the 2017 Wilhelm Award Winner I (Invited Talks)**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 406

Matthew Neurock, Chair  
Robert J. Davis, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 160a:** Sulfur Poisoning of SCR Catalysts — **Yasser Jangjou, William S. Epling**

**12:55 Paper 160b:** Overlayer Catalysts: Convincing Ourselves That the Observed Change Is Real — **Joseph H. Holmes**

**1:20 Paper 160c:** Generating Novel Compounds through Bioprivileged Molecules — **Brent H. Shanks**

**1:45 Paper 160d:** Interfacial Perimeter Sites in Au-TiO<sub>2</sub> Systems — **Alex Prokofjevs, Mayfair C. Kung, Harold H. Kung**

**2:10 Paper 160e:** Catalysis Researchers Caused Climate Change: What Can We Do to Reverse It? — **Christopher W. Jones**

**2:35 Paper 160f:** Insights into Catalytic Oxidation and Reduction Reactions at Metal/Solution Interfaces — **Matthew Neurock, Ashwin Chemburkar**

**(161) Intellectual Property for Practicing Engineers: Patents and Trade Secrets**

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 320

Charles Collins-Chase, Co-Chair  
Lauren Dowty, Co-Chair  
David Holt, Co-Chair

**Sponsored by:** Chemical Engineering & the Law Forum

**12:30 Paper 161a:** Practical Aspects of Patent Law for Chemical Engineers — **Peter Jay**

**12:50 Paper 161b:** IP Considerations in Government Contracting — **David Holt**

**1:10 Paper 161c:** How to Identify and Protect Trade Secrets — **Charles Collins-Chase, Lauren Dowty, Paul Townsend**

**(163) Managing Yourself: Reinventing Yourself for Your Next Role (Workshop)****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 331

Donna Bryant, Co-Chair  
Quinta Nwanosike Warren, Co-Chair**Sponsored by:** Management Division**12:30** Introductory Remarks**12:40** Auditing Yourself and Your Career Presentation**1:00** Auditing Yourself and Career Workshop**1:30** Branding & Selling Yourself Presentation**1:50** Branding & Selling Yourself Workshop**2:40** Concluding Remarks**(164) Materials Synthesis and Processing with Compressed or Supercritical Fluids****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 306

Christopher L. Kitchens, Chair  
Steven R. Saunders, Co-Chair**Sponsored by:** High Pressure**12:30 Paper 164a:** Stabilization of Water-in-CO<sub>2</sub> (W/C) Microemulsions with Hydrocarbon Cosurfactant — **Lei Bao**, Yang Chen, Dongdong Hu, Ling Zhao, Tao Liu, Weikang Yuan**12:50 Paper 164b:** Measurement of Glass Transition Point of Polymers Under Carbon Dioxide Using Transmitted Light Intensity — **Hiroaki Matsukawa**, Takafumi Endo, Shiho Isono, Yuichiro Shimada, Masakazu Naya, Atsushi Shono, Katsuto Otake**1:10 Paper 164c:** Supercritical Extraction for Obtaining Kinetic Data for the Catalytic Polymerization of Pyrene — **William Lamie**, Mark C. Thies, David A. Bruce**1:30 Paper 164d:** Thermo-Hydrodynamic Behavior of Coflowing Fluids in Microfluidic Supercritical Antisolvent Processes — **Fan Zhang**, Arnaud Erriguible, Samuel Marre**1:50 Paper 164e:** Laboratory-Scale Research of Non-Catalyzed Supercritical Alcohol Process for Continuous Biodiesel Production — **ASO Hassan**, Joseph D. Smith**2:10 Paper 164f:** Conversion of Magnesium Oxide to Chlorartinite with CO<sub>2</sub> and Resulting Increased Water Resistance — **Christopher L. Kitchens**, Roque Góchez, Jim Wambaugh**(165) Mixing in Rheologically Complex Fluids****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 334

Li Xi, Chair  
Quan Yuan, Co-Chair**Sponsored by:** North American Mixing Forum**12:30 Paper 165a:** Experimental and CFD Studies of a New Continuous Process for Mixing of Complex Non-Newtonian Fluids — **Simona Migliozi**, Robert Sochon, Luca Mazzei, Panagiota Angeli**12:55 Paper 165b:** Elastic Flow Compartments in Stirred Tanks — **Markus Kolano**, Matthias Kraume**1:20 Paper 165c:** Flow of Fluids with Evolving Rheology in Open Pipes and Static Mixers — **Emilio J. Tozzi**, William A. Hartt, Lori A. Bacca, Setareh Shahsavari, Matthew Laird, Robert Johnson**1:45 Paper 165d:** Optimizing Agitation in Suspension Polymerizers — **Richard K. Grenville**, Jason G. Giacomelli, Benjamin Boyer**2:10 Paper 165e:** Influence of Mixing Rate and Temperature during the up-Scaling of Emulsified Cosmetic Products — **Andrea Suaza**, Alvaro Orjuela**2:35 Paper 165f:** Experimental and Computational Studies of the Fluid Dynamic Behaviour of Liquid-Solid Mixtures in Agitated Vessels — **Giovanni Meridiano**, Weheliye Hashi Weheliye, Luca Mazzei, Panagiota Angeli**(166) Modeling of Interfacial Systems****Monday, Oct 29, 12:30 PM**

Omni William Penn Hotel, Conference Center B

Patricia Taboada-Serrano, Chair  
Ateeque Malani, Co-Chair**Sponsored by:** Interfacial Phenomena**12:30 Paper 166a:** Water Structure on Mica Surfaces: Synergistic Insights from Experiments and Molecular Simulations — **Sapna Sarupria**, Jiarun Zhou, Nurun Nahar Lata, Brittany Glatz, Will Cantrell**12:45 Paper 166b:** The Surprising Mechanism for Wettability Alteration By Non-Ionic Surfactants — **Soumik Das**, Fardin Khabaz, Quoc P. Nguyen, Roger T. Bonnecaze**1:00 Paper 166c:** Intrinsic Analysis of Fluid Interfaces Involving Ionic Liquids — **Miguel Jorge**, György Hantal, M. Natália D. S. Cordeiro, Iuliia Voroshylova, Marcelo Segal, Sofia Kantorovich, Christian Schröder**1:15 Paper 166d:** Computational Design of New Classes of Chemoresponsive Liquid Crystalline Systems — **Tibor Szilvási**, Nanqi Bao, Karthik Nayani, Huaizhe Yu, Nicholas L. Abbott, Manos Mavrikakis**1:30 Paper 166e:** Grand Canonical Monte Carlo Simulations of Electrical Double Layer Potential Profiles in Nanopores — **Patricia Taboada-Serrano**, Evan Ney, Chia-Hung Hou**1:45 Paper 166f:** Searching for Ideal Structure-Directing Agents in Colloidal Copper Nanocrystal Synthesis — **Zihao Chen**, Kristen Fichthorn**2:00 Paper 166g:** Exploiting Unique Properties of Liquid-Gas Interfaces for Efficient Gas Absorption and Separation: Insights from Molecular Dynamics — **Dmitry Lapshin**, Andrey Gromov, Eleanor Campbell, Lev Sarkisov**2:15 Paper 166h:** Molecular Dynamics Simulations Reveal Single-Stranded DNA (ssDNA) Forms Ordered Structures upon Adsorbing Onto Single-Walled Carbon Nanotubes (SWCNTs) — **Kevin R. Hinkle****2:30 Paper 166i:** Modelling of Interfacial Tension and Adsorption of Inhomogeneous Systems with Classical Density Functional Theory — **Edgar Luis Camacho Vergara**, Xiaodong Liang, Georgios M. Kontogeorgis**2:45 Paper 166j:** Using Molecular Simulation to Study the Interfacial Properties of CO<sub>2</sub>/Water/Silica Systems — **Adam R. Rall**, **Jeffrey R. Errington****(167) Nanofabrication and Nanoscale Processing II****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 310

Jung-Sheng Wu, Chair  
Shohreh Hemmati, Co-Chair**Sponsored by:** Nanoscale Science and Engineering Forum**12:30 Paper 167a:** Twenty Years of Metal Nanoparticle Synthesis Using Biotemplates — **Michael T. Harris**, Shohreh Hemmati, Oluwamayowa Adigun**1:00 Paper 167b:** Theoretical and Experimental Study of Germanium Nanoparticle Formation in a Controlled Nucleation Gas Phase Process — **Lukas Wergen**, Maximilian Domschke, Wolfgang Peukert**1:15 Paper 167c:** Tuning the Optical, Catalytic, and Physical Properties of CuO Nanosheets Using Organic Functional Groups — **Zachary Fishman**, Yulian He, Ke Yang, Brandon Ortiz, Chaolun Liu, Julia Goldsamt, Victor S. Batista, Lisa Pfefferle**1:30 Paper 167d:** Role of Mixing and Solution Phase Nitric Oxide Concentration on the Morphology of Silver Nanowires Synthesized By Polyol Process — **Prachi Kate**, **Amol Kulkarni****1:45 Paper 167e:** Spatial Atomic Layer Deposition By "Air Hockey" Design for Dielectric Multilayer Optical Films — **John A. Grasso**, Nicholas Oliveira, Brian G. Willis**2:00 Paper 167f:** Direct Biomineralization and Integration of Heterostructured Nanomaterials into Quantum Dot Sensitized Solar Cells — **Abdolhamid Sadeghnejad**, Li Lu, Christopher J. Kiely, Steven McIntosh**2:15 Paper 167g:** Monitoring Seed Formation Dynamics of Bulk-Nucleated Vapor-Solid-Solid Germanium Nanowires Via Resistance Measurements — **Benjamin Richards**, Tobias Hanrath**(168) Nanomaterials for Biological Application II****Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 412

Cerasela Zoica Dinu, Chair  
Jungbae Kim, Co-Chair**Sponsored by:** Nanomaterials for Applications in Energy and Biology**12:30 Paper 168a:** Enzyme-Based Antimicrobial Nanoconjugates — **Xia Wu**, Seok-Joon Kwon, Domyoung Kim, Jungbae Kim, **Jonathan S. Dordick**Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AICHEvents app.



**12:52 Paper 168b:** Nanobiocatalytic Antifouling in Wastewater Treatment Via Quorum Quenching — **Jungbae Kim, Kyung-Min Yeon, Inseon Lee**

**1:10 Paper 168c:** Nano-Bio-Catalysts for Enzymatic Biofuel Cells — **Su Ha, Tsai Garcia-Perez, Jungbae Kim**

**1:32 Paper 168d:** Rational Design of Mimic Multi-Enzyme Systems in Hierarchically Porous Biomimetic Metal-Organic Frameworks — **Xiao Liu, Wei Qi, Yuefei Wang**

**1:43 Break**

**1:53 Paper 168e:** Surface Active Biological Agents for Fabrication of Functional Materials for Biomedical Applications — **Ping Wang**

**2:15 Paper 168f:** Engineering Nanoscale Protein Scaffolds with Modular Functionalities — **Wilfred Chen**

**2:37 Paper 168g:** Characterizing Micellar Assembly of Oligonucleotides with Polyelectrolytes — **Alexander E. Marras, Matthew V. Tirrell**

**2:48 Paper 168h:** The Binary Effect on Drug-Resistant Bacteria of Polymeric Vesicles Appended By Proline-Rich Amino Acid Sequences and Inorganic Nanoparticles — **Nicole Bassous, Thomas J. Webster**

**2:59 Paper 168i:** Generation of Plasmonic Nanoparticles in an Amino Acid Incorporated Hydrogel for Detection of Low Doses of Ionizing Radiation — **Karthik Pushpavanam, Subhadeep Dutta, Tomasz Bista, Eric Boshoven, Stephen Sapareto, Kaushal Rege**

#### (169) New Developments in Computational Catalysis I

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 402

Shaama Mallikarjun Sharada, Chair  
Bryan Goldsmith, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 169a:** A Density Functional Theory Approach to Electrocatalytic Reaction Barriers — **Michael J. Janik**

**1:00 Paper 169b:** The Influence of Local Environment on Theoretical Calculations of Adsorption and Reaction for Catalyzed Reactions — **Alexis T. Bell**

**1:18 Paper 169c:** Tackling the Inverse Design Problem in Quantum Chemistry — **Daniel S. Lambrecht**

**1:36 Paper 169d:** Computational Alchemy to Drive Searches for Catalysts through Materials Space — **Charles Griego, Karthikeyan Saravanan, John A. Keith**

**1:54 Paper 169e:** Synergistic Application of XPS and DFT to Investigate Metal Oxide Surface Catalysis — **Quang Thang Trinh, Kartavya Bhola, Prince N. Amaniampong, Francois Jerome, Samir H. Mushrif**

**2:12 Paper 169f:** Maximal Predictability Approach for Identifying the Right Descriptors for Electrocatalytic Reactions — **Vaidish Sumaria, Dilip Krishnamurthy, Venkatasubramanian Viswanathan**

**2:30 Paper 169g:** Understanding Structure-Property Relationships in Catalysts By Using Cluster Expansions — **Chenyang Li, Tim Mueller**

#### (170) Particle Breakage and Communion Processes

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 413

Ecevit Bilgili, Chair  
Priscilla Hill, Co-Chair  
Sarang Oka, Co-Chair

**Sponsored by:** Particle Production and Characterization

**12:30 Paper 170a:** Insights from Microhydrodynamic Modeling of Nanomilling in a Wet Stirred Media Mill — **Ecevit Bilgili, Paulina Alvarez, Naveen Yaragudi, Meng Li, Afolawemi Afolabi**

**12:51 Break**

**1:12 Paper 170c:** Surface Dynamics of Micronized Active Particles — **Vibha Puri, Jag Shur, Robert Price, Ajit Narang**

**1:33 Paper 170d:** An Investigation into the Performance of an Industrial-Scale Roll Mill — **Karl Jacob, James F. Koch, Ben Freireich, Madhusudhan Kodam**

**1:54 Paper 170e:** Relation between Particle Structure, External Geometric Interaction, and Breakage Selectivity — **Kerry Johanson**

**2:15 Paper 170f:** Attrition in Submerged Jetting Region in Fluidized Bed — **Yeook Arrington, Ben Freireich, Reddy Karri, Ray Cocco**

**2:36 Paper 170g:** Dust Dispersion Particle Breakage: Classification Based on Brittleness Index — **Pranav Bagaria, Qiang Li, Ashok G. Dastidar, Chad Mashuga**

#### (171) Pharmaceutical Process Development and Pilot Plants

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 336

Onkar Manjrekar, Chair  
Vaibhav Kelkar, Co-Chair

**Sponsored by:** Pilot Plants

**12:30 Paper 171f:** Rapid Process Development - Bridging the Gap from Early Formulation Design to Integrated Continuous Drug Product Manufacture for a Dry Granulation Process — **Marcus O'Mahony, Steven Dale, Greg Connelly**

**12:55 Paper 171b:** Developing a Loss-in-Weight Feeder Design Space Based on Performance and Material Properties — **Tianyi Li, James V. Scicolone, Benjamin Glasser, Fernando J. Muzzio**

**1:20 Paper 171c:** Distillation in the Pharmaceutical Industry — **Rita Galan**

**1:45 Paper 171e:** Maintenance Management for the Sensor Network in Continuous Pharmaceutical Systems — **Sudarshan Ganesh, Francesco Rossi, Zoltan K. Nagy, G. V. Rex Reklaitis**

**2:10 Paper 171d:** Leveraging Mechanistic Models for Scale up and Optimization of Lyophilization — **Arnesh Palanisamy, Sachin Sharma, Surbhi Bagri, Gertjan Otjes, Afrouz Yousefi, Sushil Kisan Kurade, Bhushan Subhash Yeola, Sumitra Ashok Pillai, RaviChandra Palaparthi**

**2:35 Paper 171a:** Incorporation of Process Intensification Options in a Fed-Batch Cell Culture Manufacturing Platform — **Vennie Tee, Christopher Racicot, Jason Dempsey, Paul Reynolds, Misbah Anwar, Patrick Hossler**

#### (172) Rational Catalyst Design II

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 403

Matteo Cargnello, Chair  
Matthew Kale, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 172a:** Statistically Guided Synthesis of Mov- Based Mixed Oxide Catalysts for Ethane Partial Oxidation — **Juan Jimenez, Kathleen Mingle, Cun Wen, Jochen Lauterbach**

**12:50 Paper 172b:** Periodic Trends in the Morphology, Charge Distribution, and Energetics of Oxygen Vacancies on Doped MoO<sub>3</sub> (010) — **Tej S. Choksi, Jeffrey Greeley**

**1:10 Paper 172c:** DFT Study on the Catalytic Activity of Oxo-Centered Trimetallic MOF Building Units for Ethane Oxidation to Ethanol — **Melissa Barona, Sol Ahn, Omar K. Farha, Randall Q. Snurr**

**1:30 Paper 172d:** Highly Efficient Single Pt (Au) Atom Catalysts for Preferential Oxidation of CO (PROX) — **Sufeng Cao, Maria Flytzani-Stephanopoulos, Jilei Liu**

**1:50 Paper 172e:** Modified Nano-Size  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Supported Ga<sub>2</sub>O<sub>3</sub> with Improved Performance for Non-Oxidative Propane Dehydrogenation — **Nikita Dewangan, Madhav Sethia, Sonali Das, Hidajat Kus, Sibudjing Kawi**

**2:10 Paper 172f:** Design of Ni-Based Intermetallic Compounds to Promote C-H Bond Cleavage and Control C-C/C=C Bond Activation in the Dehydrogenation of Light Hydrocarbons — **Yang He, Yuanjun Song, Siris Laursen**

**2:30 Paper 172g:** Studying Sub Nano-Meter Ensemble Effects on Selective Hydrogenation Utilizing the  $\gamma$ -Brass Phase Crystal Structure — **Anish Dasgupta, Haoran He, Randall J. Meyer, Michael Janik, Robert Rioux**

#### (173) Reaction Chemistry and Engineering I

**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 404

Heather Mayes, Chair  
Milad Abolhasani, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 173a:** Solvent Reaction Coordinate for an S<sub>N</sub>2 Reaction — **Christian Leitold, Christopher J. Mundy, Marcel D. Baer, Gregory K. Schenter, Baron Peters**

**12:51 Paper 173b:** Importance of Simultaneous Reduction of Gas and Surface Mechanisms in Capturing Dominant Kinetic Features — **Devi Veerappan, Karthik Ramanathan, Niket S. Kaisare**

**1:12 Paper 173c:** A Kinetic Study of the Ethylene Oligomerization over a Nibea Catalyst — **Gabriel Seufftelli, Fernando Resende**

**1:33 Paper 173d:** Evaluation of the Thermal Decomposition Products of 2-Nitrotoluene — **Wen Zhu, Chad Mashuga**

**1:54 Paper 173e:** Modeling of Fast Cycling NO<sub>x</sub> Storage and Reduction – Effect of Reductants, Thermal Effect, and HC-Intermediate Mechanism — *Allen Wei-Lun Ting, Michael Harold, Vemuri Balakotaiah*

**2:15 Paper 173f:** Study on the Competitiveness of Homogeneous Molecular Catalysis for the Continuous Valorization of CO<sub>2</sub> in Organic Solvents — *Johann-Kilian Schnoor, Marcel A. Liao*

**2:36 Paper 173g:** Investigating the Effect of Acids and Halides on Direct Synthesis of Hydrogen Peroxide — *Pranjali Priyadarshini, David W. Flaherty*

#### (174) Solar Energy for Power Generation and Chemical Processing I

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 324

Alexandre Yokochi, Chair  
Nick AuYeung, Co-Chair  
Wojciech Lipinski, Co-Chair  
Peter Kreider, Co-Chair

**Sponsored by:** Solar Energy for Power Generation and Chemical Processing

**12:30 Paper 174a:** Revisiting Efficiency Limits of Solar Thermochemical Fuel Production By Non-Stoichiometric Ceria-Based Redox Cycling — *Sha Li, Vincent Wheeler, Peter Kreider, Wojciech Lipinski*

**12:50 Paper 174b:** Experimental Framework for Evaluation of the Thermodynamic and Kinetic Parameters of Metal-Oxides for Solar Thermochemical Fuel Production — *Richard Carillo, Jonathan R. Scheffe*

**1:10 Paper 174c:** The Effects of the Paired Charge Compensating Dopant Identity in Ceria for Solar Thermochemical H<sub>2</sub>O and CO<sub>2</sub> Splitting — *Srashtasrita Das, Christopher L. Muhich*

**1:30 Paper 174d:** Computationally Accelerated Discovery and Experimental Demonstration of Materials for Solar Thermochemical Hydrogen Production — *Samantha L. Millican, Iryna Androschuk, Charles B. Musgrave, Alan W. Weimer*

**1:50 Paper 174e:** Examining the Solar-to-Fuel Efficiency of Ceria and Perovskite Thermochemical Redox Cycles for Splitting H<sub>2</sub>O and CO<sub>2</sub> — *Christopher L. Muhich, Marie Hoes, Samuel Blaser, Aldo Steinfeld*

**2:10 Paper 174f:** Concentrated-Light Aging Techniques for High-Temperature and Solar-Energy Materials: Preliminary Results — *Konstantinos E. Kakosimos, Mohammed Al-Hashimi, Bassam Khalil, Jawad Sarwar*

**2:30 Paper 174g:** Nano-Structured Ceramic ALD Coatings to Stabilize SiC Against Oxidation in High Temperature Steam Solar Thermal Water Splitting Applications — *Amanda Hoskins, Tyler Gossett, Charles B. Musgrave, Alan W. Weimer*

#### (175) Solid-Liquid Interfaces

**Monday, Oct 29, 12:30 PM**

Omni William Penn Hotel, Conference Center A

Kai Kristiansen, Chair  
Mark Kastantin, Co-Chair

**Sponsored by:** Interfacial Phenomena

**12:30 Paper 175a:** Tuning Underwater Adhesion with Cation- $\pi$  Interactions — *Matthew A. Gebbie, Jacob Israelachvili, J. Herbert Waite*

**12:45 Paper 175b:** Towards De Novo Design of Bioadhesives with Classical DFT and Genetic Algorithm — *Alejandro Gallegos, Jianzhong Wu*

**1:00 Paper 175c:** Molecular Interactions Govern Antimalarial Drug Binding to Beta-Hematin Crystal Surfaces — *Katy N. Olafson, Jeffrey D. Rimer, Peter G. Vekilov*

**1:15 Paper 175d:** Effect of Surface Geometry on the Frictional Properties of Poly(dimethyl siloxane) — *Yunhu Peng, Lilian Hsiao*

**1:30 Paper 175e:** Morphology of Soft, Stratified and Slippery Contact — *Yumo Wang, Joelle Frechette*

**1:45 Paper 175f:** Using Elasto-hydrodynamic Deformation for Non-Contact Measurements of Flow and Particles with Graphene Nanoisland Sensors — *Charles Dhong, Darren Lipomi*

**2:00 Paper 175g:** Effect of Contact Angle Hysteresis on Solid Plugging of Condensers — *Cliff Kowall, Catherine Moran, Anne Lertola, Bingchen Wang, Lei Li*

**2:15 Paper 175h:** Understanding the Orientational Behavior of Liquid Crystals on Metal Surfaces — *Tibor Szilvási, Huaizhe Yu, Nanqi Bao, Nicholas L. Abbott, Manos Mavrikakis*

**2:30 Paper 175i:** Experimental Studies on Adsorption of Surfactants on Carbonates — *Soumik Das, Quoc P. Nguyen, Roger T. Bonnecaze*

**2:45 Paper 175j:** A Thermodynamic-Based Approach to Predict Solid-Liquid Interfacial Tension : Molecular Dynamics Simulation — *Mohamed S. AlHosani, Walter G. Chapman*

#### (176) Stem Cell and Tissue Engineering II: Engineering Tissue

**Monday, Oct 29, 12:30 PM**

Westin Convention Center, Butler

Ethan S. Lippmann, Co-Chair

Steven R. Caliari, Co-Chair

**Sponsored by:** Engineering

Fundamentals in Life Science

**12:30 Paper 176a:** Design of 3D Multi-Layered Cell-Laden Scaffolds for Tendon Tissue Engineering: The Effect of Mechanical and Biochemical Stimulation — *Chiara Rinaldi, Afsoon Fallahi, Iman Yazdi, Jessica Campos Paras, Abuduwalli Tuoheti, Ewa Kijeriska, Grissel de Santiago, Danilo Demarchi, Mario Moisés Alvarez, Nasim Annabi, Ali Khademhosseini, Wojciech Swieszkowski, Ali Tamayol*

**12:48 Paper 176b:** Neural Crest Stem Cells from Human Epidermis Skin Tissue — *Samanah moghadasi Boroujnei, Georgios Tseropoulos, Surya rajan Selvam, Pedro Lei, Stelios T. Andreadis*

**1:06 Paper 176c:** Incorporation of Hydrolytically Degradable Poly(lactic acid) in a 3D PEG Hydrogel Guides Oligodendrocyte Precursor Cell Intracellular Redox State — *Lauren Russell, Kyle Lampe*

**1:24 Paper 176d:** Low-Intensity Continuous Ultrasound Promotes Healing of Damaged Cartilage in a Pro-Inflammatory Environment — *Neety Sahu, Anuradha Subramanian, Hendrik Viljoen*

**1:42 Paper 176e:** The Role of Circulating Monocytes in the Endothelium Regeneration of Cell-Free Vascular Grafts — *Randall Smith Jr., Stelios T. Andreadis, Daniel D Swartz*

**2:00 Paper 176f:** 3D Aggregation Culture Enhances Therapeutic Outcome of Human Mesenchymal Stem Cells in Ischemic Stroke Treatment — *Xuegang Yuan, Jens Rosenberg, Yijun Liu, Ang-Chen Tsai, Sam Grant, Teng Ma*

**2:18 Paper 176g:** Surface Modifications of Small Diameter Tissue Engineered Vessels *In Vivo*: Immunological and Healing Response Variations — *Randall Smith Jr., Bita Nasiri, Tai Yi, Christopher Breuer, Stelios T. Andreadis*

**2:36 Paper 176h:** Secretome Indicators of End Tissue Quality during Human Mesenchymal Stem Cell Chondrogenesis — *Yi Zhong, Sruthi Sivakumar, Arnold I. Caplan, Jean F. Welter, Harihara Baskaran*

#### (177) Synthesis and Application of Inorganic Materials: Synthesis

**Monday, Oct 29, 12:30 PM**

David L. Lawrence Convention Center, 329

Mark A. Snyder, Chair

Xueyi Zhang, Co-Chair

Praveen K. Thallapally, Co-Chair

**Sponsored by:** Inorganic Materials

**12:30 Paper 177a:** Self-Disassembly of Two-Dimensional Zeolites in Liquid Polybutadienes — *Sanket Sabnis, Vijesh Tanna, Chao Li, Jiaxin Zhu, Vivek Vattipalli, Stephen Nonnenmann, Guan Sheng, Zhiping Lai, H. Henning Winter, Wei Fan*

**12:49 Paper 177b:** Synthesis of Metal Nanoparticles Encapsulated within Zeolites for Substrate Selective Heterogeneous Catalysis — *Hong Je Cho, Bingjun Xu*

**1:08 Paper 177c:** Novel Approach to Remove Ethanol in Commercial Y-Zeolites and Its Catalytic Activity on Paraffin Cracking — *Balasubramanian V. Vaithilingam, Abdul Majed Al Katheeri, Gnana Pragasam Singaravel, Stephane Morin, Mikael Berthod*

**1:27 Paper 177d:** Multiscale Self-Assembly of Chiral Magnetic Supraparticles with Hierarchical Structures — *Zhengzhi Mu, Nicholas Kotov*

**1:46 Paper 177e:** Colloids in Combustion: A Scalable Method to Synthesize Highly Crystalline Inorganic Nanomaterials with Tailored Porosity — *Albert A. Voskanyan, Kwong-Yu Chan*

**2:05 Paper 177f:** Universal Doping Strategy for Ordered Mesoporous Carbons Towards High Performance Energy Storage — *Zhe Qiang, Yanfeng Xia, Bryan D. Vogt*

**2:24 Paper 177g:** The Application of Green Chemistry to Enable Sustainable Manufacture of Bioinspired Nanosilica — *Joseph R. H. Manning, Siddharth V. Patwardhan*

**2:43 Paper 177h:** Leveraging Biology for Functional Inorganic Nanomaterials Development — *Nicholas Bedford*

**(178) Topical Plenary: Advances in Biosensing (Invited Talks)**  
**Monday, Oct 29, 12:30 PM**  
 Westin Convention Center,  
 Pennsylvania West

Andrew Goodwin, Chair  
 Jeffrey M. Halpern, Co-Chair

**Sponsored by:** Sensors

**12:30 Paper 178a:** Non-Invasive Disease Diagnosis Using Wearable Sensing Technologies  
 — **Hossam Haick**

**1:05 Paper 178b:** Molecular Technologies for Robust Detection of Proteins in Bodily Fluids  
 — **Hadley D. Sikes**

**1:40 Paper 178c:** Exploiting Oxygen Inhibited Photopolymerization to Control Shape, Size and Network Architecture of Functional Hydrogels As a Biosensing Platform  
 — **Katie Dongmei Li-Oakey**

**2:15 Paper 178d:** Microelectrode Cholesterol Sensing at Single Cells, Animal Tissues, and the Human Mucosa for Pre-Clinical Studies and Patient Evaluations — **James Burgess**

**(179) Getting Your Research Published (Invited Talks)**  
**Monday, Oct 29, 1:30 PM**

David L. Lawrence Convention Center,  
 303

Arthur Baulch, Chair  
 Cynthia Mascone, Co-Chair

**Sponsored by:** Publication Committee

**(180) Wilson Award Winner (Invited Talks)**

**Monday, Oct 29, 3:30 PM**  
 David L. Lawrence Convention Center,  
 327

Michael Simpson, Chair

**Sponsored by:** Nuclear Engineering Division

**3:30 Paper 180a:** Reflections from a Chemical Engineer and Life's Lessons Learned Throughout a Career  
 — **Robert S. Eby**

**(181) Networking for Nerds: How to Create Your Dream Career**

**Monday, Oct 29, 3:30 PM**  
 David L. Lawrence Convention Center,  
 330

April Grasso, Chair

**Sponsored by:** Publication Committee

**3:30 Paper 181a:** Networking for Nerds: How to Create Your Dream Career — **Alaina Levine**

**(182) Interactive Session: Applied Mathematics and Numerical Analysis**

**Monday, Oct 29, 3:30 PM**  
 David L. Lawrence Convention Center,  
 Exhibit Hall B

Ashlee N. Ford Versypt, Chair  
 Yash Puranik, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

#### ■ GENERAL APPLIED MATH, CHEMICAL, AND ENERGY TOPICS

**Paper 182a:** A Combined Graphical / Algebraic Method for Model Reduction and Analysis of Chemical Reaction Networks: Application to Atomic Layer Deposition Process — **Hossein Salami, Aisha Alobaid, Raymond A. Adomaitis**

**Paper 182b:** Optimal Solar Cell Configuration Under Partially Shaded Conditions — **Aisha Alobaid, Raymond A. Adomaitis**

**Paper 182f:** Multi-Objective Optimization of Cchp Systems Using Particle Swarm Algorithms — **Xueqiang Wang, Shuo Qiu, Jiangtao Wu**

**Paper 182g:** HPC Modeling and Simulation of Mass Transport in Wavy Falling Liquid Films — **Ming-Zhao Liu, Yi Heng, Dong-Chuan Mo, Shu-Shen Lyu**

**Paper 182h:** Autotuning with Derivative-Free Optimization — **Benjamin Sauk, Nick Sahinidis**

**Paper 182t:** An Ontology-Based Automated Generation of Training Scenarios: Development of Process Safety Rule Engine — **Dongil Shin**

#### ■ BIOCHEMICAL/BIOMEDICAL TOPICS

**Paper 182i:** Construction of a Semi-Stochastic Intracellular Signaling Model Via Global Sensitivity Analysis and Probability Density Estimation — **Dongheon Lee, Joseph Sangil Kwon, Arul Jayaraman**

**Paper 182j:** Mechanical Perturbation Approach for Treating Cardiac Arrhythmias — **Azzam Hazim, Stevan Dubljevic**

**Paper 182k:** The Impact of Glottis Opening on Drug Aerosol Delivery in a Subject-Specific Lung-Airway Model: A Numerical Study — **Yu Feng**

**Paper 182l:** Investigating LecA Binding Mechanisms with a Cellular Membrane Containing Multiple Types of Receptors Via Kinetic Monte Carlo Simulation — **Dongheon Lee, Hyun Kyu Choi, Joseph Sangil Kwon, Hung-Jen Wu**

**Paper 182m:** Rigorous Parameter Estimation for Model Validation in Oncological Systems — **Chenyu Wang, John D. Martin, Horacio Cabral, Matthew D. Stuber**

**Paper 182n:** An MCMC-Based Approach to Inferring Cell Counts in Diseased Tissue — **Muying Wang, Jason E. Shoemaker**

**Paper 182o:** Optimization in Cancer Therapeutics: Model Integration for Tumor Dynamics and Myelosuppression to Predict Chemotherapy Dosing Profiles — **Ian Dunn, Kirti M. Yenkie**

**Paper 182p:** Modeling Heat Transfer Using an Integral Equation Approach Via Green's Function: Application to Cancerous Tumor Undergoing Hyperthermia Treatment — **A. Nastasia Allred, Yung-Way Liu, J. Robby Sanders, Pedro E. Arce**

**Paper 182q:** A Modeling Framework to Characterize Kinetics, Efficacy and Toxicity of Hydroxyurea Based Treatment of Individual Sickle Cell Disease Patients — **Akantha Pandey, Robert Hannemann, Peter Kissinger, Seethal Jacob, Terry Vik, Sangtae Kim, Doraiswami Ramkrishna**

**Paper 182r:** Customized Robust Optimal Dosage Determination in the Face of Uncertainties for IVF Practices — **Apoorva Nisal, Urmila M. Diwekar**

**Paper 182s:** Metabolites from Blood Samples of Pregnant Mothers Predict Autism Risk — **Kathryn Hollowood, Jill James, Uwe Kruger, Juergen Hahn**

**(183) Interactive Session: Data and Information Systems**

**Monday, Oct 29, 3:30 PM**  
 David L. Lawrence Convention Center,  
 Exhibit Hall B

Matthew J. Realf, Chair  
 Fani Boukouvala, Co-Chair

**Sponsored by:** Data and Information Systems

**Paper 183a:** Review and Comparative Study of Nonlinear PCA Fault Detection Methods — **Weike Sun, Richard D. Braatz**

**Paper 183b:** Development of the Texas A&M Superfund Research Program Computational Platform for Data Integration, Visualization, and Analysis — **Rajib Mukherjee, Melis Onel, Burcu Beykal, Anthony H. Knap, Timothy D. Phillips, Ivan Rusyn, Michael A. Mancini, Lan Zhou, Fred A. Wright, Efstratios N. Pistikopoulos**

**Paper 183c:** Advanced Data Analytics for Process-Shop Base+Delta Sub-Model Estimation in Planning and Scheduling Decision-Making — **Robert E. Franzoi Jr., Jeffrey D. Kelly, Brenno C. Menezes, Jorge A. W. Gut**

**Paper 183d:** Blockchain Technology (other than Cryptocurrency) as a Key, Near-Future Enabler of ChE-Related Data Processing, Q&A, Supply Chains, and Data Provenance — **Anthony Skjellum**

**Paper 183e:** A Segmentation Approach for Oscillation Characterization — **Mohd Faheem Ullah, Laya Das, Sweta Parmar, Babji Srinivasan, Raghunathan Rengaswamy, Chinta Sivadurgaprasad**

**Paper 183f:** A Dead Time Compensation Approach for State Estimation of Sampled-Data Systems in the Presence of Large Measurement Delays — **Chen Ling, Costas Kravaris**

**Paper 183g:** Iterative Fault Isolation for Integrated Chemical Systems Based on Approximate Linear Model Inversion — **Xiaonan Xu, Qiang Xu**

**Paper 183j:** Hypothesis-Driven Data-Based Modeling to Study the Effect of Specialization on Hospital Performance — **Jangwon Lee, Q. Peter He**

**Paper 183k:** Dynamic Mode Decomposition Based Model Reduction for Control of Moving Boundary Problems via Approximate Dynamic Programming — **Mohammed Saad Faizan Bangi, Harwinder Singh Sidhu, Prashanth Siddhamshetty, Joseph Sangil Kwon**

**Paper 183l:** Data-Driven Optimization for Process Intensification Governed by High-Fidelity Models — **Ishan Bajaj, Shachit S. Iyer, Akhil Arora, M. M. Faruque Hasan**

**Paper 183m:** Constrained Least Square Parameter Identification Algorithms for Dual-Rate Systems with Inter-Sample Output Estimation — **Jingwei Gan, Satish J. Parulekar, Ali Cinar**

**Paper 183n:** Global Optimization of a Class of Black-Box Problems with Bounded Hessian — **Ishan Bajaj, M. M. Faruque Hasan**

**Paper 183o:** Ontology Engineering Approach to Support Process of Model Integration — **Franjo Cecelja, Linsey Koo, Edlira Kalemli**

**Paper 183p:** Prototype Study for Monitoring Flare Performance — **Albert Odell III, Qiang Xu**



**Paper 183r:** An Artificial Neural Network Approach for the Identification of Stochastic Models of Travelling Traders' Exchange Process — **Chunbing Huang**, Patrick Piccione, Federica Cattani, Federico Galvanin

**Paper 183s:** Process Data Analytics Using Deep-Learning Based Methods — **Majid Moradi Aliabadi**, Yinlun Huang, Ming Dong

#### (184) Interactive Session: Systems and Process Control

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Mona Bavarian, Chair  
Victor M. Zavala, Co-Chair

**Sponsored by:** Systems and Process Control

**Paper 184a:** Development of an Efficient Control for Smr Using Rigorous Modelling Techniques, to Improve Plant Performance, Stability, and Reliability during Feed Disturbances — **Jagan Mohan Rallapalli**, **Abdulla Saad Al-Dughaiter**

**Paper 184b:** Modified IMC-PID Controller for Stable and Time Delayed Process — **Kuldeep Sharma**, **Prabirkumar Saha**

**Paper 184c:** A Modified IMC Strategy for Unstable and Integrating Systems — **Debanjan Ghosh**, **Prabirkumar Saha**

**Paper 184d:** Leveraging Open Source, Big Data and the Cloud for Chemical Process Control — **Benjamin Rizkin**, Ryan L. Hartman

**Paper 184e:** A Synthesis Framework for Structure Constrained Thermally Coupled Distillation Sequences Including Divided Wall Columns — **Haotian Ye**, Xiong Zou, Weixuan Zhu, Yang Yang, Hong-guang Dong

**Paper 184f:** A Novel Robust Kalman Filter Algorithm Using Incremental PID Controller for Model Uncertainties — **Min-kyung Lee**, **Byeong Eon Park**, **Jun-Hyung Ryu**, In-Beum Lee

**Paper 184g:** Simultaneous Uncertainty Reduction and Control of Hydraulic Fracturing — **Abhinav Narasingam**, Joseph Sangil Kwon

**Paper 184h:** Non-Linear Model Predictive Control of Module Temperature in Photovoltaic System — **Dheeraj Kumar**, Arun K. Tangirala

**Paper 184i:** Discrete-Time Nonlinear Observer-Based Globally Linearizing Control of a PEM Fuel Cell — **K. Sankar**, Amiya K. Jana

**Paper 184j:** Robust Model Predictive Control for Smart Grid Integrated with Solar Power and Energy Storage System Under Regular and Abnormal Loads — **Yu Yang**, Hen-Geul Yeh, Son Doan

**Paper 184k:** Data Analysis, Optimization and Control Methodologies on a Fluid Catalytic Cracking Unit (FCCU) for an Implementation of Real Time Optimization — **Adriana L. Rodriguez**, Carlos A M Riascos

**Paper 184l:** Feedback Predictive Control Versus Model Predictive Control for Automatically Controlling Blood Glucose Concentration — **Yong Mei**, **Derrick Rollins**

**Paper 184m:** Dual Control Framework with Multistep Ahead Prediction Model — **Yu Yang**, Anthony Perez

**Paper 184n:** Black Box Operation Optimization for Temperature Control of Basic Oxygen Furnace Process — **Yongxia Liu**, Jingyu Tang, Yuan Wang

**Paper 184o:** Optimal Control of BOF Steelmaking with Considering Energy Consumption — **Dongying Song**, Jingyu Tang

**Paper 184p:** Machine Learning Techniques for Model Identification from Historical Data for Control — **Manikandan S**, Raghunathan Rengaswamy

**Paper 184q:** Modeling and Control of Proppant Distribution of Multi-Stage Hydraulic Fracturing in Horizontal Wells — **Prashanth Siddhamshetty**, Kan Wu, Joseph Sangil Kwon

**Paper 184s:** A Monte Carlo Simulation Study to Evaluate the Limits of Prediction Accuracy for Blood Glucose Concentration — **Yong Mei**, **Derrick Rollins**

**Paper 184t:** Dynamic Optimization of Natural Gas Network with Rigorous Thermodynamics — **Kai Liu**, Lorenz T. Biegler, **Bingjian Zhang**, Qinglin Chen

**Paper 184u:** Modelling and MPC Design of Mineral Column Flotation Process — **Yahui Tian**, Fei Liu, **Stevan Dubljevic**

**Paper 184v:** Multiple Phase Shifted Chirp Signals for Rapid Impedance Estimation: Applications in Diagnosis of Electrochemical Systems — **Resmi Suresh**, Sathish Swaminathan, Raghunathan Rengaswamy

**Paper 184w:** Development of Advanced Model-Based Controllers for Optimal Load-Following Operation of the Supercritical Pulverized Coal Power Plants — **Parikshit Sarda**, Elijah Hedrick, Katherine Reynolds, Emily Tomer, Benjamin P. Omell, Stephen E. Zitney, **Debansu Bhattacharyya**

**Paper 184x:** Recurrent Neural Network-Based Model Predictive Control for Continuous Pharmaceutical Manufacturing — **Wee Chin Wong**, Jiali Li, **Xiaonan Wang**

**Paper 184z:** Smart Constrained Model Predictive Control — **Su Liu**, Jinfeng Liu

**Paper 184aa:** Simultaneous Scheduling of Refinery Manufacturing and Pipeline-Based Multi-Oil Product Distribution — **Li Yu**, **Qiang Xu**

#### (185) Interactive Session: Systems and Process Design

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Monica Zanfir, Chair  
Xiaonan Wang, Co-Chair  
Charles C. Solvason, Co-Chair

**Sponsored by:** Systems and Process Design

#### ■ 10A00 A POSTER SESSION PROCESS DESIGN

**Paper 185a:** Single & Multi-Objective Optimizations Using Parallelized Process Simulators — **Trevor Rice**, Mingder Lu

**Paper 185b:** Development of a Spatio-Temporal Multi-Objective Optimisation Model for Multi-Product Oil Palm Value Chains — **John Frederick D. Tapia**, Sheila Samsatli

**Paper 185c:** Optimal Synthesis of Reaction Networks for the Manufacture of Benzaldehyde from Toluene Via the P-Graph Methodology — **Jean Pimentel**, Andres Argoti, Ivan Gil, Istvan Heckl, Botond Bertok, Ferenc Friedler, Juan Carlos Garcia-Ojeda

**Paper 185d:** Simulation Approach for Natural Gas Sweetening Using Mixed Amines — **Mohammed S. Ba-Shammakh**

**Paper 185e:** Impact of Biomass Densification on the Overall Economics of Renewable Gasoline and Diesel Production — **Sampath Gunukula**, William J. DeSisto, M. Clayton Wheeler

**Paper 185f:** A Novel Conceptual Design for Simultaneous Production of Biodiesel and Glycerol Carbonate from Soybean Oil — **Cuixia Xu**, **Qiang Xu**

**Paper 185g:** Spray Drying System Modelation for Orange (*Citrus sinensis*) Juice Drying Using Open Foam — **Andrés Ramos Sr.**, **Ricardo Cogua Barrera**, **Luis Alberto Figueroa Sr.**

**Paper 185h:** Tackling the Challenges/ Limitations Posed By Heat Exchanger Network in Work-Heat Exchange Network Synthesis — **Sajitha K. Nair**, **Iftekhar A. Karimi**

**Paper 185i:** Uncertainty Analysis Including Safety, Environmental and Economic Performance of Chemical Processes — **Andrea Paulina Ortiz-Espinoza**, Karen de Jesús Guillén-Cuevas, Arturo Jiménez-Gutiérrez, Vasiliki Kazantzi, Fadwa T. Eljack, **Mahmoud M. El-Halwagi**, **Nikolaos Kazantzi**

**Paper 185k:** Design of Carbon-Hydrogen-Oxygen Symbiosis Networks with CO<sub>2</sub> Monetization and Footprint Constraints — **Marc Panu**, Kevin Topolski, Sarah Abrash, **Mahmoud M. El-Halwagi**

**Paper 185l:** Integrating Mass and Heat in the Synthesis of Carbon-Hydrogen-Oxygen Symbiosis Networks — **Kevin Topolski**, Marc Panu, Luis Fernando Lira-Barragan, José María Ponce-Ortega, **Mahmoud El-Halwagi**

**Paper 185n:** Optimal Design of PHAs Plants with Alternative Substrates — **Fernando Ramos**, Claudio Delpino, Marcelo Villar, **Maria Soledad Diaz**

**Paper 185o:** Optimizing Energy System Design Using a Parallel Tabu Search Algorithm — **Art Vollbrecht**, K. V. Camarda

**Paper 185p:** Optimization of CO<sub>2</sub> Remediation through Use of a Novel Decomposition Algorithm — **Hayden Boline**, K. V. Camarda

**Paper 185q:** Computer-Aided Tools for Process and Product Design — **Anjan Kumar Tula**, Mario Richard Eden, Rafiqul Gani

**Paper 185r:** A Simple and Fast Reduction Method Applied to the Large Scale Distillation Sequences Synthesis — **Weixuan Zhu**, Xiong Zou, **Haotian Ye**, **Yang Yang**, Hong-guang Dong

**Paper 185s:** Optimal Design of Gas Supply Chains Including Shale with Economic and Environmental Criteria — **Josselin Colin-Robledo**, Sergio Ivan Martinez-Guido, Luis Fernando Lira-Barragan, **José María Ponce-Ortega**, Medardo Serna-Gonzalez



**Paper 185t:** Multi-Scale Simultaneous Parameter Estimation in Rate-Based Processes — **Paul Akula, John C. Eslick, Debangsu Bhattacharyya, David C. Miller**

**Paper 185u:** Development of a One-Dimensional Bubbling Fluidized Bed Model for a Coal-Fed Chemical Looping Combustion Fuel Reactor — **Chinedu O. Okoli, Andrew Lee, Anthony P. Burgard, David C. Miller**

**Paper 185v:** A New Optimization-Based Computer-Aided Molecular and Mixture Design (OptCAMD) Framework — **Lei Zhang, Qilei Liu, Linlin Liu, Jian Du, Rafiqul Gani**

## 10A00 B POSTER SESSION DESIGN AND OPERATION UNDER UNCERTAINTY

**Paper 185w:** The Optimization of Integrated Energy System Under Uncertainty Based on Genetic Algorithm — **Shuo Qiu, Xueqiang Wang, Jiangtao Wu**

**Paper 185x:** Application of Sequential Design of Experiments (SDoE) to a MEA-Based CO<sub>2</sub> Capture Pilot Plant — **Joshua C. Morgan, Benjamin P. Omell, Michael S. Matuszewski, Christine Anderson-Cook, Charles Tong, Debangsu Bhattacharyya, David C. Miller, Muhammad Ismail Shah, Thomas De Cazenove**

**Paper 185y:** Process Synthesis and Simultaneous Minimization of Inherent Risk — **Andreja Nemet, Zdravko Kravanja**

**Paper 185z:** Quantitative Risk Assessment of Soft Sensor Predictions Using Fast PDF Estimation — **Francesco Rossi, Sudarshan Ganesh, Qinglin Su, Linas Mockus, Gintaras Reklaitis**

**Paper 185aa:** Development of Artificial Lift Infrastructure Plan Under Endogenous and Exogenous Uncertainties — **Zuo Zeng, Selen Cremaschi**

**Paper 185ab:** Bayesian Design of Experiments for Fault Detection and Isolation — **Evan K. Stefanidis, Kyle A. Palmer, George M. Bollas**

**Paper 185ac:** Optimization System for Biomass Supply Chain Under Seasonal Variation — **Ken-Ichiro Sotowa, Hiroki Kondo, Jesus Rafael Alcantara-Avila, Toshihide Horikawa**

## 10 A00 C POSTER SESSION PROCESS INTENSIFICATION

**Paper 185ad:** Design of Optimal Multistage Heat Exchange Networks — **Nadir Ziyatdinov, Artem Bezrukov, Ilya Emelyanov, Denis Kubanov**

**Paper 185ae:** Experimental and Numerical Investigation to Develop the Ultrasound Assisted Oxidative Desulfurization (UAOD) Process in a New Continuous-Flow System — **Masoud Rahimi, Shahrokh Shahhosseini, Salman Movahedrad, Mohammad Amin Sobati**

**Paper 185af:** Model-Based Analysis and Optimization of a Semi-Lean MBC Process for Natural Gas Sweetening — **Ven Chian Quek, Javier Rodriguez, Nilay Shah, Benoit Chachuat**

**Paper 185ag:** Process Intensification of Hydrogen Production Systems — **Secgin Karagoz, Theodore Tsotsis, Vasilios Manousiouthakis**

**Paper 185ah:** Heat Integration and Controllability Analysis of Heat Exchanger Networks — **Nabil Abdel Jabbar, Ibrahim Masoud, Rachid Chebbi, Muhammad Qasim**

## (186) Interactive Session: Systems and Process Operations

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Chrysanthos E. Gounaris, Chair  
Pieter Schmal, Co-Chair

**Sponsored by:** Computers in Operations and Information Processing

**Paper 186a:** Optimization-Based Retrofit of a Cryogenic Air Separation Unit for Flexible Operation — **Artur M. Schweidtmann, Pascal Schäfer, Adrian Caspari, Hagen Seele, Pascal Padberg, Christoph Offermanns, Adel Mhamdi, Alexander Mitsos**

**Paper 186b:** Planuling: A Hybrid Planning and Scheduling Optimization to Schedule Slow and Plan Fast Processes — **Jeffrey D. Kelly, Robert E. Franzoi Jr., Brenno C. Menezes, Jorge A. W. Gut**

**Paper 186c:** GoNDEF: A New Exact Method to Generate All Non-Dominated Points of Multi-Objective Mixed-Integer Linear Programs — **Metin Turkay, Seyyed Amir Babak Rasmi**

**Paper 186d:** Data-Driven Robust Optimization with Principal Component Analysis and Kernel Smoothing — **Chao Ning, Fengqi You**

**Paper 186e:** Validation of CFD Prediction Accuracy of VOC Generation Rate for Cost-Effective Design of VOC Recovery Equipment — **Xidong Hu, Manabu Kumagami, Shaoxiang Qian, Nobuhiro Yamada, Masahiro Kawasaki, Takashi Iitsuka, Syuichi Oguro**

**Paper 186f:** Process Design Quality for the Success of Industrial R&D at SABIC — **Zheng Liu, Brain Peng, Blamurali Nair**

**Paper 186g:** A Multi-Objective MILP Model for Spatio-Temporal Design and Operation of Multi-Product Oil Palm Value Chains — **John Frederick D. Tapia, Sheila Samsatli**

**Paper 186h:** Numerical Analysis of Effect of Diaphragm Structure Based on Thermo-Electro-Magneto-Hydrodynamics Coupling Model in Magnesium Electrolysis cell — **Cheng-Lin Liu, You-Fa Jiang, Jin Xue, Jian-Guo Yu**

**Paper 186i:** Integrated Design and Control of Intensified Membrane-Based Hydrogen Production Via Methane Steam Reforming — **Alexios S. Kyriakides, Spyros S. Voutetakis, Simira Papadopolou, Panos Seferlis**

**Paper 186j:** Scale up Design Optimization of Pressure Swing Adsorption Processes for Gas Separation — **Daeho Ko**

**Paper 186k:** Scale up Design Optimization of a Membrane Module for Gas Separation — **Daeho Ko**

**Paper 186l:** Solving Real-World Natural Gas Gathering Systems — **Russell Burnett, Charles C. Solvason, Michael Sellers**

**Paper 186m:** On the Temporal Evolution of the Material Stress Profile in a Supercritical Pulverized Coal Boiler Under Load-Following Operation — **Katherine Reynolds, Elijah Hedrick, Parikshit Sarda, Emily Tomer, Benjamin P. Omell, Stephen E. Zitney, Debangsu Bhattacharyya**

**Paper 186n:** Optimization of Single-Well CO<sub>2</sub> Injection for Enhancement of Tight Oil Production — **Guofan Luo, Christine Ehlig-Economides, Michael Nikolaou**

**Paper 186o:** A Novel Methodology to Optimize the Operation of Combined Cooling Heat and Power Systems — **Sayyed Faridoddin Afzali, Vladimir Mahalec**

**Paper 186p:** Simultaneous Crude Procurement Planning and Movement Scheduling for Petroleum Refineries — **Honglin Qu, Qiang Xu**

**Paper 186q:** Dynamic Production Planning and Scheduling for an Chemical Plant — **Min Chen, Qiang Xu, Wang Zhenlei**

**Paper 186r:** Sustainable Strategic Planning for a National Natural Gas Energy System Accounting for Unconventional Sources — **Esbeydi Villicaña-García, José María Ponce-Ortega**

**Paper 186s:** A Multi-Objective MILP Model for Planning, Design and Operation of Biomass Supply Chains – Capturing the Trade-Offs within the Food-Energy-Water-Environment Nexus — **Sheila Samsatli**

**Paper 186t:** Data-Driven Multi-Period Planning Model and Global Optimization for Entire Petroleum and Petrochemical Operations — **Wei Khang Ooi, Jie Li, Xin Xiao, Yong Qiao, Baoguo Zhao, Guangming Du, Xin Su, Hongwei Liu**

## (187) Poster Session: Advances in Fossil Energy R&D

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Dushyant Shekhawat, Chair

**Sponsored by:** Advances in Fossil Energy R&D

**Paper 187b:** Ultra-Deep Desulfurization of Low-Sulfur Gasoline By Selective Adsorption of Trace Mercaptans over Supported Metal Oxides — **Cuiting Yang, Guang Miao, Zhong Li, Jing Xiao**

**Paper 187c:** Catalytic Adsorptive Desulfurization (CADS) of Diesel Using Industrial-Grade MCM-41 — **Xiong Dai, Guang Miao, Zhong Li, Jing Xiao**

**Paper 187d:** Economic and Environmental Implications of the Transition from CO<sub>2</sub>-Enhanced Oil Recovery to Saline Aquifer Sequestration — **Matthew Jamieson, Gregory Cooney**

**Paper 187f:** Evolution of CO<sub>2</sub> Storage Capacity Associated with Geochemical Reactions in Subsurface — **Wei Jia, Ting Xiao, William Ampomah, Nathan Moodie, Brian McPherson**

**Paper 187g:** Quantitative Analysis of the Influence of Capillary Pressure on Geologic Carbon Storage Forecasts. Case Study: CO<sub>2</sub>-EOR in the Anadarko Basin, Texas — **Nathan Moodie, William Ampomah, Wei Jia, Jason Heath, Brian McPherson**

**Paper 187h:** Measurement and Calibration of Self-Sealing Rate of Fractures in Geological CO<sub>2</sub> Storage: Case Study of a Natural Analog — **Vivek Patil**, Brian McPherson, Edward Trujillo, Hyukmin Kweon

**Paper 187q:** New Data and Models to Avoid Cryogenic Solids Formation in LNG Production — **Arman Siahvashi**, Saif ZS. Al-Ghafri, Brendan F. Graham, Eric F. May

**Paper 187i:** An Innovative Technology for the Production of Value Added Chemicals Using Fischer Tropsch Synthesis — **Syed Ali Zeeshan Gardezi**

**Paper 187j:** Strongly Coupled Co@CoO<sub>x</sub> Nanoparticles and Layered Perovskite As a Highly Stable and Efficient Cathode for Solid Oxide Electrolysis Cells — **Yongdan Li**

**Paper 187k:** Bimetallic Pd-Cu Catalysts for CO<sub>2</sub> Hydrogenation to Methanol — **Xiao Jiang**, Xiaowa Nie, Xinwen Guo, Krista S. Walton, Chunshan Song

**Paper 187l:** Energy Analysis of Non-Aqueous Solvents (NASs) for CO<sub>2</sub> Capture Process — **Aravind V. Rayer**, Paul Mobley, Vijay Gupta, Jak Tanthana, Mustapha Soukri, Marty Lail, S. James Zhou

**Paper 187m:** Microwave Assisted Lignin Depolymerization Using Deep Eutectic Solvents — **Pranjali Muley**, Dorin Boldor, Jian Shi, Bert C. Lynn

**Paper 187n:** Enhanced Gasification Reactor Designs for Maximizing Gas-Particle Interaction — **Quang Truong**, Srujan Rokkam, Matt Flannery

**Paper 187o:** Modeling the Decomposition Kinetics of the Gas Hydrates in Porous Medium — **Avinash V. Palodkar**, Amiya Kumar Jana

**Paper 187p:** Modeling Phase Equilibrium with Wong-Sandler Mixing Rule for Ternary CO<sub>2</sub>/H<sub>2</sub>/C<sub>2</sub>H<sub>6</sub> Hydrates — **Niraj Thakre**, Amiya Kumar Jana

**(188) Poster Session: Bioengineering**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

Adam Melvin, Chair  
J. Andrew Jones, Co-Chair  
Rajib Saha, Co-Chair  
Amy J. Karlsson, Co-Chair  
Yongku Cho, Co-Chair  
Ryan Summers, Co-Chair

**Sponsored by:** Bioengineering

## ■ SYNTHETIC BIOLOGY

**Paper 188a:** Multiplexed Perturbation of Gene Expression with CRISPR Induces Epistasis and Deters Bacterial Adaptation to Antibiotics — **Peter Otoupal**, William Cordell, Madeleine Sittton, Vismaya Bachu, Anushree Chatterjee

**Paper 188b:** Bioprocess of Crude Cell Extract Preparation for Bacterial Cell-Free Protein Synthesis System — **Yong-Chan Kwon**, Jeehye Kim, Caroline E. Copeland

**Paper 188c:** Biosensor Based Engineering of Synthetic Pathways for Biomanufacturing — **Niju Narayanan**, Scott Patrick Henelly, Naresh Pandey, Taraka Dale, Ramesh Kumar Jha

**Paper 188d:** Tunable Crispr-Based Transcriptional Control in *Clostridium Pasteurianum* Using dCas12a — **Rochelle Joseph**, Nicholas R. Sandoval

**Paper 188e:** Study of the Effects of Surfactants on the Brownian Motion of Fluorescent Polystyrene Beads in Silicone Oil — **Maha Yusuf**, Punng Padhy, Mohammad Asif Zaman, Michael Jensen, Lambertus Hesselink

**Paper 188f:** Designing and Screening Protein-Sensing Riboswitches in an All-*E. coli* Cell-Free Expression System — **Grace Vezeau**, Howard Salis

**Paper 188g:** Enhancing Butanol Tolerance of *Escherichia coli* Via Solo Gene Reveals Hydrophobic Interaction of Multi-Tasking Chaperone SecB — **Guochao Xu**

**Paper 188h:** Design Driven Engineering of Extracellular Sensors for the Development of Mammalian Cell-Based Therapies — **Taylor Dolberg**, Patrick S. Donahue, Joseph J. Muldoon, Kelly A. Schwarz, Joshua N. Leonard

**Paper 188i:** Expanding the N-End Rule Pathway of Protein Degradation in *Escherichia coli* — **Aditya M. Kunjapur**, George M Church

**Paper 188j:** Peptide Nucleic Acid Antibiotics Design and Screening Against Multidrug Resistant Bacteria — **Thomas Aunins**, Colleen Courtney, Kristen Eller, Jocelyn Campos, Keesha Erickson, Anushree Chatterjee

**Paper 188l:** Extractable Microwell Arrays for Screening Microbial Interaction Networks — **Ryan Hansen**, Andre van der Vlies, Niloy Barua, Priscila Guzman, Tom Platt

**Paper 188m:** Construction of Genetic Logic Gates Using Transcriptional Interference — **Antoni E. Bordoy**, Nolan O'Connor, Anushree Chatterjee

**Paper 188n:** Nanoparticle-Mediated Transgene Expression and Silencing in Agriculturally-Relevant Plants — **Gozde Sultan Demirel**, Huan Zhang, Juliana Matos, Roger Chang, Linda Chio, Brian Staskawicz, Markita Landry

**Paper 188o:** Engineering Synthetic Consortia Inspired By the Rumen Microbiome — **Michelle O'Malley**, Sean P. Gilmore, Xuefeng Peng

**Paper 188p:** Critical Analysis of Methodologies Based on Fluxomics for Identifying Active Elementary Flux Modes — **Caroline Satye Martins Nakama**, José Gregório Cabrera Gomez, Galo Antonio Carrillo Le Roux

**Paper 188q:** Engineering a Synthetic Methanol Utilization Pathway in *Escherichia coli* for Examining Metabolic Bottlenecks Associated with Developing Synthetic Methylophs — **R. Kyle Bennett**, Eleftherios T. Papoutsakis

**Paper 188r:** Rapid Discovery of Lanthipeptides and Glycocins through Pathway Refactoring in *Escherichia coli* — **Hengqian Ren**, Subhanip Biswas, Sherri Ho, Wilfred A. van der Donk, Huimin Zhao

**Paper 188s:** Thermodynamic Characterization of Click Nucleic Acid-DNA Binding for Biosensing — **Heidi R. Culver**, Xun Han, Benjamin D. Fairbanks, Christopher N. Bowman

## ■ BIOCATALYSTS & BIOBASED PRODUCTS

**Paper 188t:** PEGylated Hyaluronic Acid Hydrogels with Tunable Properties — Byungduk Kim, Jinku Kim

**Paper 188u:** Comparative Genomic Analysis for Two *Methanothermobacter* Species Isolated from the Reactor for Thermophilic and Hydrogenotrophic Bio-Methanation of CO<sub>2</sub> — **Byoung Seung Jeon**, Mungi Hong, Kowoon Ju, Sung Min Han, Hyunjin Kim, Okkyung Choi, **Byoung-In Sang**

**Paper 188v:** Bio-Ionic Liquid Conjugated Gels (BiGEL): Hemostatic, Antimicrobial and Highly Adhesive Hydrogel — **Iman Noshadi**, **Vaishali Krishnadoss**, Leah Filardi, Tyler Hannah

**Paper 188w:** Customized, 3D-Printed Devices for Immune Cell Migration across Porous Membranes — **Marcus Bunn**, Dana Spence

**Paper 188x:** A 3D Printed, Two-Compartment Model for Antibiotic Susceptibility Testing — **Andrew A. Heller**, Dana Spence

**Paper 188y:** Theranostic Optical Fibers for Tumor Treatment and Sensing — **Ai Lin Chin**, Rong Tong

**Paper 188z:** Development of a Modular Pathway Optimization Toolbox for *Synechococcus Elongatus* PCC 7942 — **Nicholas A. Kaplan**, Alexandra M. Adams, Xin Wang, J. Andrew Jones

**Paper 188aa:** Design of a Foaming Formulation for Application in Remediation of Soils Contaminated with Hydrocarbons — **Mariana Ramirez-Morales**, Victor-Hugo Ocadiz-Salazar, Tomás-Eduardo Chávez-Miyauchi, Juan-Rodrigo Salazar

**Paper 188ab:** Combinatorial Approach for Effective Entrapment of Model Enzyme Glucose Oxidase in Hyaluronin Acid Nanogel — **Jordan Chapman**

**Paper 188ac:** Algal-Assisted Nutrient Removal of Municipal Wastewater in a Sequential Batch Reactor — **Carlise Sorenson**, Carlos Zamalloa, Bo Hu

**Paper 188ad:** Stiffness of Engineered Substrate Alters Cellular Function in Liver and Contributes to Fibrosis — **Michael Moeller**, Senthilkumar Thulasigam, Srivatsan Kidambi

**Paper 188ae:** Overcome the Challenges of Balancing Complex Rosmarinic Acid Biosynthetic Pathway By Utilizing Microbial Co-Cultures — **Haoran Zhang**, Zhenghong Li, Xiaonan WANG

**Paper 188af:** Exploring and Enhancing the Activity and Substrate Specificity of Amine Dehydrogenases — **Robert D. Franklin**, Conner Mount, Bettina Bommarius, Andreas S. Bommarius

## ■ CELL CULTURE ENGINEERING

**Paper 188ag:** Yeast Hydrolysate Fractions and the Impact on Monoclonal Antibody Production — **Josephine Chiu**, William Buggele, Melissa Good, Taha Salim, Wai Lam Ling

**Paper 188ah:** Engineering Pancreatic Islet Organoids from Human Pluripotent Stem Cells — **Nadine Humphrey**

**Paper 188ai:** Modeling and Simulation of Engineered Cardiac Tissue Under Forced Perfusion — **Tyler Corrales**, Mario Oyanader, **Steffano Oyanader**

**Paper 188aj:** A Microfluidic Approach to Quantify Three-Dimensional Directed Cellular Migration of Highly Invasive Cancer Cells — **Sharif M. Rahman, Joshua M. Campbell, Ian Schneider, Adam Melvin**

**Paper 188ak:** Oxidative Stress and Antioxidant Protection in Human Pulmonary Cells — **Jordan A. Hoops, Timothy M. Brenza**

**Paper 188al:** Differentiated Transcriptome Profile of 3T3-L1 Adipocytes in 3-D *in Vitro* Culture — **Paul Turner, Michael Garrett, Sean Didion, Amol V. Janorkar**

**Paper 188am:** Increase Recombinant Bax Expression By Inducing *E. coli* Cells at Oxygen Limiting Condition with a Constant kLa — **Yi He**

**Paper 188an:** On the Evaluation of the Efficiency of the Chemotherapeutic Agent Gemcitabine on 3D Polymer Based Pancreatic Cancer Models of Various Extracellular Matrix Compositions — **Stella Totti, Mark Allenby, Susana Brito Dos Santos, A. Mantalaris, Eirini Velliou**

## ■ METABOLIC ENGINEERING

**Paper 188ao:** Improved n-Butanol Production of *Clostridium Cellulovorans* by Integrated Metabolic, Evolution and Process Engineering — **Zhiqiang Wen, Yu Jiang, Sheng Yang**

**Paper 188ap:** Expression, Purification, and Characterization of the New Recombinant Crotonamine Isoform from the Venom Gland of *Crotalus Oreganus Helleri* on Antimicrobial Activity — **Roland Montemayor, Dr. Montamas Suntravat, Dr. Elda Sanchez**

**Paper 188aq:** Butanol Production from Cellulose By *Clostridium Cellulovorans adhE2* in a Two-Stage pH-Regulated Fermentation Process — **Xin Liu, Teng Bao, Shang-Tian Yang**

**Paper 188ar:** Genome-Scale Metabolic Model of *Chromochloris*, an Emerging Model Organism for Sustainable Fuel Production — **Alexander Metcalf, Nanette R. Boyle**

**Paper 188as:** Towards the *In Vivo* Biosynthesis of *Psilocybe* Natural Products — **Alexandra M. Adams, Nicholas A. Kaplan, J. Andrew Jones**

**Paper 188at:** Enhancing Phenol Biosynthesis By Exploiting Modular Co-Culture Engineering Strategies — **Xiaoyun Guo, Zhenghong Li, Jing Wang, Juan Chala, Xiaonan Wang, Haoran Zhang**

**Paper 188au:** Deep Scanning Mutagenesis on the *Escherichia coli* Genome Help Understand Principles of Protein Engineering Towards Strain Optimization — **Alaksh Choudhury, Jacob Fenster, Olivier Tenaillon, Ryan T. Gill**

**Paper 188av:** Combining Metabolic Flux Analysis and Proteomics to Decipher Regulation of Carbon Fixation in Cyanobacteria — **Nathaphon Yu King Hing, Feiyan Liang, Peter Lindblad, John A. Morgan**

**Paper 188aw:** Improved Heterologous Production of Salicylate 2-O- $\beta$ -D-Glucoside Through *E. coli* metabolic System Modification — **Ruiquan Qi**

**Paper 188ax:** An Integrative Approach of Metabolic Network and Bioprocess Modeling in the Strain Design for Succinic Acid Production — **Albert Tafur Sr., Jorge M. Gómez, Andrés Fernando González-Barrios**

**Paper 188ay:** Optimization of PHA Production by *Pseudomonas* using <sup>13</sup>C-Metabolic Flux Analysis — **Rafael D. Oliveira, Vânia Novello, José Gregório Cabrera Gomez, Galo A. C. Le Roux**

**Paper 188az:** Engineering *Yarrowia Lipolytica* As a Platform for Production of Plant Secondary Metabolites — **Huan Liu, Yongkun Lv, Monireh Marsafari, Peng Xu**

**Paper 188ba:** Engineering a  $\beta$ -Ketoadipate Biosensor in *Pseudomonas Putida* and Evolution of Aromatic Catabolism Pathway for Biomanufacturing — **Niju Narayanan, Naresh Pandey, Scott Patrick Henelly, Christopher Johnson, Gregg T. Beckham, Taraka Dale, Ramesh Kumar Jha**

**Paper 188bb:** Peroxisome Engineering for Improved Heterologous Biochemical Production — **Michael Spagnuolo, Meredith Bailey, Murtaza Shabbir Hussain, Mark Blenner**

**Paper 188bc:** Photocatalytic Production of the Jet Fuel Limonene in *Synechococcus* Sp. PCC 7002 — **Cara L. Sake, Fiona Davies, Nanette R. Boyle**

**Paper 188bd:** Cell-Free Production of Isobutanol — **Matthew Wong, Jian Zha, Mamta Gupta, Kamran Jawed, Marlene Belfort, Mattheos A.G. Koffas, Georges Belfort**

**Paper 188bf:** Thermostable Laci for Inducible Expression in *Geobacilli* — **Matilda Delgado, Kang Wu**

**Paper 188bg:** Development of *Actinobacillus succinogenes* 130Z As a Biotechnology Host for Succinic Acid Production — **Dianna Long, Cheryl Immethun, Rajib Saha**

## ■ MODELING & DOWNSTREAM PROCESSING

**Paper 188bh:** Viral Filter Fouling By Monoclonal Antibody Under Seemingly Mild Oxidizing Conditions — **Michael Iammarino, Lauren Rockwell, Sunitha Kandula, Nihal Tugcu**

**Paper 188bi:** Charge-Switch Membranes for the Rapid Isolation of microRNA — **Mayuri Singh, Rachael Cohen, Stephanie McCalla**

**Paper 188bj:** Optimising the Morphology and Flow Attributes of 3D Scaffold Perfusion Systems for Effective Cell Deposition — **Vineeth Siripuram, Abhineet Nigam, Anirban Roy, Siddhartha Moullick**

**Paper 188bk:** Heavy Metal Recovery from Waste Water Using Yersiniabactin Adsorbed over Activated Carbon — **Girish Swayambhu**

**Paper 188bl:** Development of Synthetic Perfluorinated Photobioreactor System for Simultaneous CO<sub>2</sub> separation and Promotion of Microalgae Growth and Productions — **Yu-Hsiang Lee**

**Paper 188bm:** Role of Electrical Fields in the Pre-Treatment of Polyacrylamide Gels for Enhancing Protein Separations — **Anfal Haris, J. Robby Sanders, Pedro E. Arce**

## ■ PROTEIN SCIENCE & ENGINEERING

**Paper 188bn:** Development of an Electrochemical Biosensor for Lactate Concentration Determination in Sweat — **Hsiao-Ying Tang, Chelsea Monty**

**Paper 188bo:** Engineering Bispecific Antibodies to Synergistically Inhibit Tumor Metastasis — **Huilin Yang, Wentao Wang, Michelle Bahri, Jamie Spangler**

**Paper 188bp:** Combining Yeast and Virion Protein Displaying Platforms for Antibody Drug Discovery — **Patrick J. Krohl, Harsh Kapadia, Santi Balza, Jamie Spangler**

**Paper 188bq:** Truncation and Characterization of the Caffeine *N*-Demethylase Reductase from *Pseudomonas Putida* CBB5 — **Shelby Brooks, Ryan M. Summers**

**Paper 188br:** Expression of SDS-Resistant Chitinase, AsChi61, Identified from *Aeromonas Schubertii* Using Enzymomics Analysis — **Chung-Yu Wu, Yu-Ping Liu, Jeen-Kuan Chen, Chao-Lin Liu**

**Paper 188bs:** Site-Specific Conjugation of Scfv Using the Nucleotide Binding Site — **Franklin Mejia, Nur Mustafaoglu, Michael Canonico, Basar Bilgicir**

**Paper 188bt:** Integrating Non-Printed Materials into 3D-Printed Devices for Quantitative Biological Measurements — **Cody Pinger, Dana Spence**

**Paper 188bu:** Self-Interactions of a Virus Glycan Shield — **Eric Ogharandukun, Abeyratne-Perera Hk, Chandran Preethi**

**Paper 188bv:** Facilitating Protease Engineering Using Golden Gate (GG) Assembly — **Carl A. Denard, Natalie McGinnis, Rasha Yaghi, Brent L. Iverson**

**Paper 188bw:** Methods for High Throughput Fabrication and Screening of Protein-Based Materials — **Carolyn Mills, Erika Ding, Bradley D. Olsen**

**Paper 188bx:** Engineering Protein Secretion Tags in *Yarrowia Lipolytica* and Its Industrial Application — **Wanqi Sun, Peng Xu**

**Paper 188by:** Microparticles for Skin Wound Healing — **Daniel Smith, Sutapa Barua**

**Paper 188bz:** Microsphere Immunoassay and Cell Tracking Velocimetry to Diagnose Iron-Related Disorders in Point-of-Care Applications — **Mitchell Weigand**

**Paper 188ca:** Colicin Production Using Cell-Free Protein Synthesis to Control Persister Cell Formation — **Xing Jin, Weston Kightlinger, Yong-Chan Kwon, Seok Hoon Hong**

**Paper 188cb:** Selective Targeting of Acute Lymphoblastic Leukemia (ALL) Via CD22 Targeting Liposomal Nanoparticles — **Jaeho Shin, Baksun Kim, Basar Bilgicir**

**Paper 188cc:** NiO<sub>2</sub>, Pt, and Cu Surface Modifications of a Glassy Carbon Electrode for Electrocatalysis of Amino Acids — **Christian A. Tooley, Charles Gasperoni, Micaela Schones, Jeffrey M. Halpern**

**Paper 188cd:** Electrochemical Biosensors for Pollutant Detection — **Ariel Furst, Matthew Francis**



**Paper 188ce:** A Multifunctional Versatile 3D Melanoma Model for Rapid Micro-Needle Based *in Situ* detection of Disease Specific Biomarkers — *Stella Totti, Keng Wooi Ng, Guoping Lian, Tao Chen, Eirini Velliou*

**Paper 188cf:** Investigation of Lectin-Functionalized Surfaces As Biosensors Towards Pathogen Capture Using Azlactone-Based Block Copolymers As a Reactive Platform — *Mohammadali Masigol, Niloy Barua, Bradley Lokitz, Ryan Hansen*

**Paper 188cg:** Ultrasensitive Microna Detection for Disease Diagnosis — *Burcu Ozay, Stephanie McCalla*

**Paper 188ch:** A Study of the Effect of Nutraceuticals on Healthy and Interleukin  $\beta$ -1 Induced Osteoarthritis in Bovine Articular Chondrocytes — *Mahmoud Amr, Alia Mallah, Haneen Abusharkh, Bernard J. Van Wie, Nehal I. Abu-Lail, Arda Gozen, Juana Mendenhall, Vincent Idone*

**Paper 188ci:** Developing a Robust Reporter System to Evaluate and Improve Amber Suppression in Yeast — *Jessica T. Stieglitz, Haixing P. Kehoe, James Van Deventer*

**Paper 188cj:** Lanosterol Reverses Alpha-Crystallin Aggregates Induced by Different Denaturation Processes — *Li Ke, Daniel Forciniti*

**Paper 188ck:** Effect of Methanol and Glycerol on the Structure of Plasma Protein Solutions — *Paul Praveen Nakka, Daniel Forciniti*

**Paper 188cl:** Single Molecule Investigation of TALE Protein's Genome-Wide Target Search in Live Cells — *Surbhi Jain, Saurabh Shukla, Charles M. Schroeder, Paul Selvin, Huimin Zhao*

**Paper 188cn:** Antimicrobial Activity and Cytotoxicity of Buforin II Immobilized on Magnetite Nanoparticles — *Jessica Giovanna Perez Pineda, Juan Carlos Cruz Jimenez, Carolina Muñoz-Camargo*

**Paper 188co:** Enzyme Immobilization: Predictive Structure-Function Relationships for Effective Enzyme-Linker-Surface Complexes — *Maxwell Hilbert, Adam Beitz, Siva Dasetty, Sapna Sarupria, Mark Blenner*

**Paper 188cp:** Palmitate Directly Interacts with IRE1 $\alpha$  to Induce Its Activation — *Amrita Oak, Christina Chan*

**Paper 188cq:** Molecular Dynamics Simulations of Protein Refolding in Deep Eutectic Solvents — *Samal Kaumbekova, Dhawal Shah*

**Paper 188cr:** A Molecular Dynamics Study of Carbohydrate Preferential Interactions with Small Proteins — *Theresa Cloutier, Chaitanya Sudrik, Hasige Sathish, Bernhardt L. Trout*

**Paper 188cs:** In silico/in Vitro Combined Study of Lamin A/C Protein Mutations and Their Effects on Biomechanical and Molecular Properties — *Erik Laurini, Domenico Marson, Maurizio Fermeglia, Silvia Boccardo, Orfeo Sbaizero, Thomas Lanzicher, Luca Puzzi, Daniele Borin, Valentina Martinelli, Suet N. Chen, Luisa Mestroni, Carlin S. Long, Matthew R.G. Taylor, Patrice Lee, Sabrina Prcl*

**Paper 188ct:** Mixtures of Tense and Relaxed State Polymerized Human Hemoglobin Regulate Oxygen Affinity and Tissue Construct Oxygenation — *Donald Belcher, Uddyalok Banerjee, Christopher Baehr, Kritopher Richardson, Pedro Cabrales, François Berthiaume, Andre Palmer*

**Paper 188cu:** Development and Characterization of Tunable Zein-Based Tissue Adhesives — *Aimé A. Cuéllar Monterrubio, Everardo Gonzalez Gonzalez, Regina Vargas Mejía, Christian Mendoza Buenrostro, Mario Moisés Alvarez, Grissel Trujillo-de Santiago*

**Paper 188cv:** Engineering Ligand-Regulated Adhesion Proteins Targeting ICAM-1 — *Liang Fang, J. Vincent Price, Eric T. Boder*

**Paper 188cw:** Identifying the Atomistic Features That Enhance the Rate of Methyl-Transfer Catalysis of Ketol-Acid Reductoisomerase — *Natasha Seelam, Brian Bonk, James Weis, Bruce Tidor*

**Paper 188cx:** Optimization of Redox Reporter Molecule Sensing Parameters for Square Wave Voltammetry — *Tugba Yilmaz, Martin K. Kimani, Edgar D. Goluch*

**Paper 188do:** Contributions of the C-Terminus and Mutations to  $\alpha_{2a}^{\text{r}}$  Activity and Stability — *Kirsten Swonger, Anne S. Robinson*

**Paper 188dp:** Media Supplementation Strategies for Improving Stability and Glycan Quality in Mabs — *Anne S. Robinson, Evan Wells*

**Paper 188dq:** Isolation and Characterization of Giant Plasma Membrane Vesicles Containing  $\alpha_{2a}^{\text{r}}$  and Gas for Optical Biosensing — *Daniel Oseid, Anne S. Robinson*

## ■ SYSTEMS & QUANTITATIVE BIOLOGY

**Paper 188cz:** Bioelectrochemical Reduction of Carbon Dioxide to Methane and Acetate Using Thermophilic Microorganisms — *Okkyoung Choi, Hyejeong Song, Byoung Seung Jeon, Byoung-In Sang*

**Paper 188da:** Data-Driven Analysis of Antimicrobial Resistance of Foodborne Pathogens in Six States of USA — *Nina Zhang, Emily Liu, Alexander Tang, Martin Ye, Kevin Wang, Qian Jia, Zuyi (Jacky) Huang*

**Paper 188db:** Flocculation Induction on Microalgae Consortia Cultures with Organic Wastes — *Omar S. Castillo, Christian A Cabrera, Stephanie Acosta, J. Rubén Rodríguez, Vicente Peña-Caballero, Luz María Landa*

**Paper 188dd:** Development of 3D Culture Systems Requiring No Extrinsic Gas Exchange — *Julia Lin, Clayton S Jeffryes*

**Paper 188de:** Computational Modeling of Biofilm Chemotaxis Induced By a Carbon-Rich Plume in Sediments — *George E. Kapellos, Nicolas Kalogerakis, Patrick S. Doyle*

**Paper 188df:** Balancing Biophysical Tradeoffs to Drive Cellular Reprogramming — *Kate E. Galloway, Kimberly Babos, Justin Ichida*

**Paper 188dg:** A modeling and experimental investigation of the correlation between cell size nanoparticle uptake at the single-cell level — *Md Shahinuzzaman, Jawahar Khetan, Sutapa Barua, Dipak Barua*

**Paper 188di:** Networks, Oscillations and Evolution: A Computational Approach — *Matthew Putnins, Ioannis P. Androulakis*

**Paper 188dj:** Multi-Omics Analysis Reveals That Co-Exposure to Phthalates and Metals Disturbs Urea Cycle and Choline Metabolism — *Dimosthenis Sarigiannis, Nafsika Papaioannou, Nikos Kapretos, Aikaterini Gabriel, Emilie Distel, Eliandre De Oliveira, Spyros Karakitsios, Martine Aggerbeck, Robert Barouki*

**Paper 188dk:** Application of Cybernetic Control Variables in the Modeling of Lipid Metabolism in Mammalian Systems — *Lina Aboulmouna, Shakti Gupta, Mano R. Maurya, Frank T. DeVilbiss, Shankar Subramaniam, Doraiswami Ramkrishna*

**Paper 188dl:** Exploring the Role of G6PC2 Under Hyperglycemia Using a Novel  $\beta$ -Cell Metabolism Model — *Mohsin Rahim, Richard O'Brien, Jamey D. Young*

**Paper 188dm:** Integrative Analysis of Glycosylation Networks Using Transcriptomics and Glycomics Data Sets — *Yusen Zhou, Theodore Groth, Sriram Neelamegham*

**Paper 188dn:** Investigating Signal Integration in Bacteria Chemotaxis — *Jingyun Yang, Ravi Chawla, Rachit Gupta, Nitesh Sule, Pushkar Lele, Arul Jayaraman*

## (189) Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Jim Pfaendtner, Chair  
Heather Mayes, Co-Chair  
Sapna Sarupria, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**Paper 189a:** The Effects of Ionic Correlation and Surface Polarization on Electrostatic Inter-Colloid and Inter-Emulsion Interactions — *Meng Shen*

**Paper 189b:** Probing Enzyme Catalyzed Hydrolysis of Cellulose in Ionic Liquids Using Enhanced Sampling Techniques — *Sarah Alamdari, Jim Pfaendtner*

**Paper 189c:** Computational Study of Electrochemical Reduction of CO<sub>2</sub> on Transition Metal /p-Block Hybrid Nanocatalysts — *Sahithi Ananthaneni*

**Paper 189d:** From Metal to Plastic: Computer-Assisted Material Design for Marine Engine Non-Structural Components — *Erik Laurini, Maurizio Fermeglia, Alberto Marinò, Serena Bertagna, Vittorio Bucci, Sabrina Prcl*

**Paper 189e:** Stay Double, Stay Homologous: Combined Computational/Experimental Approaches to RAD51/ssDNA Interactions in DNA Damage Repair — *Domenico Marson, Erik Laurini, Suzana Aulic, Maurizio Fermeglia, Sabrina Prcl*

**Paper 189f:** Influence of Basis Set on the Electronic Structure and Physico-Chemical Properties of the Cerium Tribromide and the Cerium Trichloride: Two Lanthanide Compounds — *Jean Baptiste Fankam Fankam*



**Paper 189g:** Multi-Scale Simulations of Biomacromolecules for Design of Biomaterials — **Phrashaanna Ammu**, Joshua Condon, Phillip Taylor, Arthi Jayaraman

**Paper 189h:** Binding Rates of Polyaromatic Hydrocarbons during Soot Formation: Insights from Reactive Molecular Dynamics — **Eirini Goudeli**, Christopher J. Hogan Jr.

**Paper 189i:** Capturing Non-Ideal Surfactant/Nanoparticle Interfacial Structure with Variable Coverage Molecular Simulations — **Junwoong Yoon**, Zachary Ulissi

**Paper 189j:** Challenges and Strategies of Modeling Extra-Framework Metal Cations in Zeolites from First-Principles: Knowledge Learned from Cationic Iron Exchanged in SSZ-13 — **Sichi Li**, William F. Schneider

**Paper 189k:** Molecular Simulations of Liquid-like Assemblies of Intrinsically Disordered Proteins — **Gregory L. Dignon**, Wenwei Zheng, Young C. Kim, Jeetain Mittal

**Paper 189l:** Competitive Adsorption of Toxic Gases in a Humid Environment: Insights from Density Functional Theory — **N. Scott Bobbitt**, Randall Q. Snurr

**Paper 189m:** CO<sub>2</sub> Adsorption in Nickel Based Metal Organic Framework Ni-DABCO: A Density Functional Theory and Grand Canonical Monte Carlo Study — **Orlando A. Mulero Flores**, Paul Meza-Morales, Maria Curet-Arana

**Paper 189n:** A Comparison of Crystalline and Icosahedral Order in Ag<sub>6</sub>Cu<sub>4</sub> and CuAu Alloys — **Brittany Gonzalez**, Solene Bechelli, Caroline Desgranges, Jerome Delhommelle

**Paper 189o:** Molecular Dynamics Simulation of Modified Nafion 117 Based Anion Exchange Membrane Fuel Cell: Transport and Nanophase-Segregated Structure Properties — **Seung Soon Jang**, **Charles Caliendo Jr.**

**Paper 189p:** Efficient Generation of Polymer Amorphous Structure By Reverse-Mapping from Beads-Spring to Full-Atomistic Model — **Hiroya Nitta**, Taku Ozawa

**Paper 189q:** Structural and Vibrational Properties of a Si- and Se- Induced 216-Atom Quasi-Random Ingaas — **Haili Jia**

**Paper 189r:** Modeling Rosette Nanotubes Using the Martini Forcefield — **Vyshnavi Karra**, Hicham Fenniri, Francisco R. Hung

**Paper 189s:** Conformal Sites Model for Adsorbed Films on Energetically Heterogeneous Surfaces — **Kaihang Shi**, Erik E. Santiso, Keith E Gubbins

**Paper 189t:** Screening of Bio-Based Plasticizers for Poly(vinyl chloride) and Poly(lactic acid) Via Atomistic Simulations — **Marcel Balçik**, Hüsamettin D. Özeren, M. Goktug Ahunbay, J Richard Elliott

**Paper 189u:** A Combined Molecular Dynamics and Experimental Study of an Imidazolium Based Ionic Liquid Electrolyte Solution for Low Temperature Applications — **Marisa E. Gliege**, Yifei Xu, Wendy J. Lin, Zuofeng Zhao, Stella D. Nickerson, Hongyu Yu, Lenore L. Dai

**Paper 189v:** Biasing High-Dimensional Free-Energy Landscapes for the Detection of Stable Clusters in Self-Assembling Systems — **Arushi Prakash**, Christopher Fu, Jim Pfandtnr

**Paper 189w:** GPU Accelerated Experiment Directed Metadynamics for Scattering Profile Biasing — **Andrew White**, Rainier Barrett

**Paper 189x:** Aggregation Behavior of 1-n-Dodecyl-3-Methylimidazolium Octylsulfate Biamphiphilic Ionic Liquid in Aqueous Solution — **Utkarsh Kapoor**, Jindal K. Shah

**Paper 189y:** Composition Effect on the Nucleation Process in CuNi Systems — **Solène Bechelli**, Brittany Gonzalez, Caroline Desgranges, Jerome Delhommelle

**Paper 189z:** Temperature Influence on Potassium Chloride Solution and Sodium Chloride Solution Structure — **Junsheng Yuan**, Fei Li

**Paper 189aa:** Predicting Point Defect Concentrations in Complex, Disordered Oxides — **Samantha L. Millican**, Ann M. Deml, Alan W. Weimer, Aaron M. Holder, Vladoan Stevanovic, Charles B. Musgrave

**Paper 189ab:** Reweighting Molecular Simulation Configurations for Rapid Force Field Parameterization — **Richard A. Messerly**, Michael R. Shirts, S. Mostafa Razavi

**Paper 189ac:** Importance of Molecular Conformations on Dipole Moment and Thermophysical Properties Estimation — **Minh Nguyen Vo**, Michael Call, Cliff Kowall, J. Karl Johnson

**Paper 189ad:** Computer-Aided Description of Materials Stability at the Nanoscale — **Michael G. Taylor**, Giannis Mpourmpakis

**Paper 189ae:** Dissipative Particle Dynamics Simulations of Reactant Transport through Multicompartment Micelle Nanoreactor — **SeungMin Lee**, Connor Callaway, Nicholas Bond, Kayla Hendrickson, Aditya Kuntamukkula, Seung Soon Jang

**Paper 189af:** Study of the Effect of a LiOH Layer over the Reactivity of Lithium Metal Anode — **Maria Stefany Angarita-Gomez**, Perla B. Balbuena

**Paper 189ah:** The Influence of Pore Structure on Transport in Lyotropic Liquid Crystal Membranes — **Benjamin J. Coscia**, Michael Shirts

**Paper 189ai:** Combinatorial Computational Studies Towards Advancing Lithium Ion Battery Technologies — **Yudhajit Pal**, Gang Wu, Johannes Hachmann

**Paper 189cn:** High-Throughput in silico Screening of Candidate Compounds for Deep Eutectic Solvents — **Yudhajit Pal**, Johannes Hachmann

**Paper 189aj:** Modeling Side Chain Conformations of Bottlebrush Polymers from iSAFT Density Functional Theory — **Yuchong Zhang**, Shun Xi, Walter G. Chapman

**Paper 189ak:** Web Applications for Rapid Characterization of Nanoporous Materials — **Benjamin Bucior**, Randall Q. Snurr

**Paper 189al:** Agglomerate Formation with Polydisperse Primary Particles in the Transition Regime — **Georgios A. Kelesidis**, Eirini Goudeli, Sotiris E. Pratsinis

**Paper 189am:** Coarse-Grained Model for Simulating the Boiling Point of Asphaltenes — **Steve Groven**, Caroline Desgranges, Jerome Delhommelle

**Paper 189an:** DFT Study on the Catalytic Activity of ALD-Grown Iron Oxide Nanoclusters for the Partial Oxidation of Methane to Methanol — **Melissa Barona**, Omar K. Farha, Joseph T. Hupp, Randall Q. Snurr

**Paper 189ao:** Conformational Mapping of Viral RNA Elements Using Atomistic Simulations — **Lev Levintov**, Harish Vashisth

**Paper 189ap:** A Molecular Dynamics Study on Interfacial Properties of NaClO<sub>4</sub>/Carbonate Electrolyte Near Graphene-Based Electrode for Na-Ion Battery — **Sungwon Park**, Eunsu Paek

**Paper 189aq:** Gating Mechanisms during Actin Filament Elongation By Formins — **Fikret Aydin**, Naomi Courtemanche, Thomas D. Pollard, Gregory A. Voth

**Paper 189ar:** Comparison of Interatomic Potentials for Interfacial Studies of Ionic Liquid Systems — **Felix Tiet**, Matt Thompson, Peter T. Cummings

**Paper 189as:** Mechanism Development for Catalyzed Ketene Production — **Charles J. McGill**, Sara Jo Taylor, Phillip R. Westmoreland

**Paper 189at:** Foyer: A Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems — **Christopher R. Iacovella**, Christoph Klein, Justin Gilmer, Andrew Z. Summers, Jana E. Black, János Sallai, Peter Volgyesi, Clare McCabe, Peter T. Cummings

**Paper 189au:** MoSDeF: A Python-Based Molecular Simulation and Design Framework — **Justin Gilmer**, Christoph Klein, János Sallai, Andrew Z. Summers, Chris Iacovella, Ákos Lédeczi, Peter Volgyesi, Peter T. Cummings, Clare McCabe

**Paper 189av:** Challenging Statistical Mechanics Approximations in Organic Crystal Thermodynamics — **Nathan Abraham**, Michael Shirts, Eric Dybeck\*

**Paper 189aw:** Molecular Modeling of Microstructure and Solubilization of Single and Multiple Micelles — **Shun Xi**, Walter G. Chapman

**Paper 189ax:** Proteins in Extreme Environments: From Understanding Life to Potential Applications — **Betul Uralcan**, Pablo G. Debenedetti

**Paper 189ay:** Applications of Chemml Program Suite in Predicting Properties of Organic Materials: A Path to Data-Driven Discovery in Chemistry — **Mojtaba Haghighatlari**, Johannes Hachmann

**Paper 189bi:** Advancing Machine Learning and Molecular Descriptor Methodologies Using the Chemml Program Suite — **Mojtaba Haghighatlari**, Johannes Hachmann

**Paper 189ba:** Benchmarks for Adsorption on Transition Metal Oxide Surfaces: A Comparison of DFT to Experimental Data for NH<sub>3</sub> on MnO(100) — **Han Chen**, David F. Cox

**Paper 189bb:** Molecular Dynamics Simulation of Mixed Aqueous Solutions of NH<sub>4</sub>Cl and (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> — **Junsheng Yuan**, Jihong Wang

**Paper 189bc:** Combining Molecular Simulation, Liquid State Theory, and Gibbs Ensemble Techniques to Study the Structure, Thermodynamics, and Phase Behavior of Polymer-Solvent Mixtures — **Thomas Gartner III, Arthi Jayaraman**

**Paper 189be:** Molecular Dynamics Simulation of Hydration and Swelling of Mixed Layer Clays — **Mahsa Rahromostaqim, Muhammad Sahimi**

**Paper 189bf:** Reactive Sorption of Sulfur Contaminants By Copper Oxide: A First-Principles Study — **Tirso Lopez-Ausens, Philippe Sautet, Dante Simonetti**

**Paper 189bg:** Colloidal Crystal Structure Analysis Using Symmetry Groups and Stochastic Optimization — **Evan Prettì, Nathan A. Mahynski, Vincent K. Shen, Jeetain Mittal**

**Paper 189bh:** Feasst: Free Energy and Advanced Sampling Simulation Toolkit — **Harold W. Hatch, Nathan A. Mahynski, Vincent K. Shen**

**Paper 189az:** Modeling the Transformation of Ethene over MFI Using a Hybrid QM/MM Strategy — **Erum Mansoor, Martin Head-Gordon, Alexis T. Bell**

**Paper 189bk:** Prediction of Phase Behavior of Mixed Solvent Electrolyte Systems Using SAFT-VRE Morse EoS — **Reza Shahryari, Mohammad Reza Dehghani**

**Paper 189bl:** Characterization of Heat Absorption and Decomposition Products for Suppressant Agent/Combustible Dust Mixtures Via TGA/DSC/MS Analysis — **Nicholas Reding, Mark B. Shiflett**

**Paper 189bm:** Measurement of the Liquid Thermal Conductivity of HFO-1336mzz(Z)(cis-1,1,1,4,4,4-hexafluoro-2-butene) By Transient Hot-Wire Method — **Shuo Qiu, Xueqiang Wang, Jiangtao Wu**

**Paper 189bn:** Thermodynamic Properties and Molecular Interactions of Azeotropic Mixtures Using Molecular Simulation and Modeling — **Dongyang Li, Hong Li, Xingang Li, Xin Gao, Li Xi**

**Paper 189bo:** Refining the Nonrandom Two-Liquid Segment Activity Coefficient Model By Applying the Association Theory — **Yifan Hao, M. R. Islam, Chau-Chyun Chen**

**Paper 189bp:** Thermodynamic Description of Shear-Induced Phase Transition in Jammed Soft Particle Glasses — **Fardin Khazaz, Michel Cloitre, Roger T. Bonnecaze**

**Paper 189br:** Isotropic-Nematic-Smectic Transition of Highly Confined Semi-Flexible Polymer Solutions — **Yeng-Long Chen, Supriya Roy, Dmytro Luzhbin**

**Paper 189bs:** Prevention of High-Temperature Hydrogen Attack in Liquid Lines By Accurate Estimation of Hydrogen Partial Pressure — **Paul M. Mathias, Garry Jacobs, Cathleen Shargay**

**Paper 189bt:** CFD Simulations for Gas Solubility Measurements with Gas-Liquid Segmented Flows — **Pradeep Vyawahare, Mark W. Vaughn, Chau-Chyun Chen**

**Paper 189bu:** Thermodynamic Modeling of Saturn Particles and Phase Behavior in Patchy Colloid Mixtures — **Yiwei Zhu, Artee Bansal, Walter G. Chapman**

**Paper 189bv:** An Ordinary Differential Equation Based Machine Learning Framework — **Luke E. K. Achenie**

**Paper 189bw:** PID Control Strategy for Thermostating and Barostating Molecular Dynamics Simulation — **Shih-Han Wang, Luke Achenie**

**Paper 189bx:** Multiscale Modeling of Actin Filaments — **Harshwardhan H. Katkar, Fikret Aydin, Tamara C. Bidone, Alyssa J. Harker, David R. Kovar, Gregory A. Voth**

**Paper 189bz:** Fluid Behavior and Interfacial Structure of Heterogeneous GO Interlayer Pores — **Xiaoning Yang, Tongfei Yu, Shuyan Liu**

**Paper 189ca:** Molecular Simulation and Experimental Study of Oxalic Acid Adsorption on Water-Feldspar Interface — **Xiaopeng Xue, Ping Li**

**Paper 189cb:** Molecular Dynamics Analysis of Membrane Proteins As Biosurfactants into Triglycerides – Water Mixtures — **Juliana Erika Cristina Cardona Jaramillo, Oscar A. Alvarez, Luke E. K. Achenie, Andrés F. González**

**Paper 189cc:** Prediction of Calcium Carbonate Wettability By Low Salinity Water Flooding Using Molecular Dynamics Simulations — **Mohamed S. AlHosani, Fernando Yrazu, Arjun V. Parambathu, Walter G. Chapman**

**Paper 189cd:** Thermodynamic Stability of Thiolate-Protected Gold Nanoclusters: From Molecular to Metallic Systems — **Michael Cowan, Michael G. Taylor, Giannis Mpourmpakis**

**Paper 189ce:** Reactive Molecular Dynamics Simulation of Disintegration of Cross-Linked Epoxy-Resin Polymers upon Atomic Oxygen Bombardment — **Chowdhury Ashraf, Aniruddh Vashisth, Adri C. T. van Duin**

**Paper 189cf:** Molecular Simulation of CO<sub>2</sub> Absorption into MCM-41 Porous Material Filled with PDMS Solvent — **Wei Shi, Jeffery Culp, David Hopkinson**

**Paper 189cg:** MD Simulation of a Magnesium Oxide Grain Boundary — **Adriaan Riet, James Van Orman, Daniel J. Lacks**

**Paper 189ch:** Atomistic Simulation of Sliding Friction between Two Silicon-Carbide Surfaces — **Nariman Piroozan, Saber Naserifar, Muhammad Sahimi**

**Paper 189ci:** QSAR Modeling for Predicting Elimination Half-Life of Industrial Chemical Compounds — **Krystalia Papadaki, Spyros Karakitsios, Dimosthenis Sarigiannis**

**Paper 189cj:** Understanding Reaction and Transport in External Electric Fields with Molecular Simulations — **Shen Tan, Yi He**

**Paper 189ck:** Electrophilic Aromatic Substitution and Intrinsic Nature of Aromaticity — **Mohamed S. AlHosani, Walter G. Chapman**

**Paper 189cl:** Prediction of Hg0 and HgCl<sub>2</sub> Adsorption Properties in UiO-66 Using Optimized Force-Fields — **Hongjian Tang, Hanjun Fang, David S. Sholl, Yufeng Duan**

**Paper 189cm:** Using Artificial Neural Networks to Model Diffusion Characteristics in Lithium Solid State Electrolytes — **Karun K. Rao, Yan Yao, Lars C. Grabow**

**Paper 189co:** Using Free Energy Perturbation (FEP) to Rank Binding Affinities for ssDNA-Wrapped Single-Walled Carbon Nanotube (SWCNTs) — **Kevin R. Hinkle, Frederick R. Phelan Jr.**

**Paper 189cp:** Screening of Nano Porous Materials for Large-Scale Molecular Separations — **Dai Tang, Grit Kuppang, Coray M. Colina, David S. Sholl**

**(190) Poster Session: Engineering Fundamentals in Life Science**

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

Abigail Koppes, Chair  
Stacey D. Finley, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**Paper 190a:** A Hidden Light – Selection of Green Fluorescent Protein That Evades an Existing Antibody Response — **Jacob Furlon, Karl E. Griswold**

**Paper 190b:** Continuous Protease Assays Using Liquid Crystal As a Reporter — **Mahbuba Jannat**

**Paper 190d:** Study of the Magnetic Properties of Glioblastoma Cancer Stem-like Cells and Non-Stem Tumor Cells Using Magnetophoresis for Label-Less Separation — **James Kim, Jeffrey J. Chalmers**

**Paper 190e:** Preservation of Therapeutic Potential of Culture Expanded Human Mesenchymal Stem Cells By Preventing a Breakdown of Cellular Homeostasis — **Xuegang Yuan, Yijun Liu, Ang-Chen Tsai, Teng Ma**

**Paper 190f:** Induction of Definitive Endoderm from Human Pluripotent Stem (hPS) Cells — **Saber Meemardoost, Natesh Parashurama**

**Paper 190g:** Peptoid-Based Coatings for Differentiation of Human Embryonic Stem Cells into Neural Cells — **Jesse Roberts, German Perez, Safiya Belbina, Michael Borrelli, Ruben M. Ceballos, Shannon L. Servoss**

**Paper 190h:** Biomolecular Rate Indicators of Human Mesenchymal Stem Cell Chondrogenesis — **Yi Zhong, Sruthi Sivakumar, Arnold I. Caplan, Jean F. Welter, Harihara Baskaran**

**Paper 190i:** Three-Dimensional Finite Element Modeling of Dynamic BMP Gradient Formation in Zebrafish Embryonic Development — **Linlin Li, Xu Wang, Adrian Buganza Tepole, David M. Umulis**

**Paper 190j:** Cell Population Balance of Cardiovascular Spheroids Derived from Human Induced Pluripotent Stem Cells — **Julie Bejoy, Yuanwei Yan, Junfei Xia, Jingjiao Guan, Yan Li**

**Paper 190k:** Understanding the Role of Central Carbon Metabolism in Myeloid and Monocytic Hematopoietic Differentiation Programs in Patient Derived HL-60 Cells — **David Dai, Andrew Yen, Jeffrey Varner**

**Paper 190l:** Reverse-Engineering Calcium Signaling in a Developing Organ — **Jeremiah J. Zartman**

**Paper 190m:** NANOG Restores the Myogenic Differentiation Potential of Senescent Myoblasts — **Aref Shahini**, Debanik Choudhury, Kalyan Vydiam, Nika Rajabian, Thy Nguyen, Pedro Lei, **Stelios T. Andreadis**

**Paper 190n:** Transport of Amyloid- $\beta$  across the Blood Brain Barrier By P-Glycoprotein: A Novel Therapeutic Target in Alzheimer's Disease — **Hope Holt**, Elizabeth Moore, Madeline Riese, Michelle Faucett, Francisco González, Melissa A. Moss

**Paper 190o:** In Situ Growth of Acetylcholinesterase-Oxime Polymer Conjugate Scavengers of Organophosphate Nerve Agent Toxicity — **Libin Zhang**, Nicholas Harris, Weihang Ji, Hironobu Murata, Krzysztof Matyjaszewski, Alan Russell

**Paper 190p:** Ultrasound Triggered Synergistic Thrombolysis Using Tpa Loaded Microbubbles for the Treatment of Acute Ischemic Stroke — **Vishnu Sunil**, Vijay Kumar Sharma, Chi-Hwa Wang

**Paper 190r:** Inherent Variability in Inflammatory Response to Shunts in the Treatment of Hydrocephalus — **Carolyn Harris**, Prashant Hariharan, Marc Del Bigio, David Limbrick, James P McAllister

**Paper 190s:** Polydopamine Nanoparticles: A Possible Strategy to Fight Against Cancer — **Celia Nieto**, Milena Vega, Gema Marcelo, Miguel A. Galán, Eva Martín del Valle

**Paper 190t:** GGL: A Natural Pharmaceutical Molecule for the Treatment of Breast Cancer — **Muhammad Raisul Abedin**, Sutapa Barua

**Paper 190u:** Encapsulation of 6-Thioguanine on Al-MOF Basolite A100 and Its Controlled Delivery — **Cole Grinnell**, Adetunji Adeniran-Adetoye, Rena Lapidus, **Alexander Samokhvalov**

**Paper 190v:** Rheological Response of Chromatin to DNA Damage — **Daniel Whitefield**, Kris Noel Dahl, Li Lan, Shelly Peyton

**Paper 190x:** Implantable Humanized Pre-Metastatic Niches Capture Microenvironmental Regulation of Disseminated Human Tumor Cells — **Ryan Carpenter**, Jun-Goo Kwak, **Jungwoo Lee**

**Paper 190y:** Increased Resistance Enhances Cell Motility — **Kaustav Bera**, Adrianna Boen, Panagiotis Mistriotis, Konstantinos Konstantopoulos

**Paper 190z:** Effects of Immune Modulation on Melanoma Progression — **Adeyinka Lesi**, Richard White, David S. Rumschitzki

**Paper 190aa:** Exploring the Metabolic Shift Associated with Cancer Hypermutation — **Jonathan L. Robinson**, Raphael Ferreira, Francesco Gatto, Jens Nielsen

**Paper 190ab:** Engineering Cancer Cells for Cancer Research — **Everardo Gonzalez Gonzalez**, Aimé A. Cuéllar Monterrubio, Grissel Trujillo-de Santiago, Mario Moisés Alvarez

**Paper 190ac:** Label-Free Interference-Based Single-Cell Phenotyping of Highly Metastatic Cancer Cells in Liquid Biopsy Applications — **Jose C. Contreras-Naranjo**, Arul Jayaraman, Victor M. Ugaz

**Paper 190ad:** Biodegradable Multilayered Nanofilms for Isolation and Recovery of Circulating Tumor Cells — **Wei Li**, Ziye Dong, Dan Yu

**Paper 190ae:** Mesenchymal Stem Cell Infiltration and Remodeling of Microfiber/Hydrogel Composites for Ligament Tissue Engineering — **Hagar Kenawy**, Aaron S. Goldstein, Dina Gadalla, Patrick Thayer

**Paper 190af:** Simulating Bacterial Infection to Trick Neutrophils into Enhancing Vaccine-Induced Immune Response — **Seth Boese**

**Paper 190ag:** Antitumor and Antioxidant Activities of Crude Proteins Extracts from Enzymatically Treated Microalgae — **Sulaiman Al-Zuhair**, Sinan Battah

**Paper 190ai:** Engineering Peptide Targeting Liposomal Drug Delivery to Improve Selectivity for HER2-Overexpressing Breast Cancer — **Baksun Kim**, Jaeho Shin, Junmin Wu, Laurie Littlepage, Basar Bilgicer

**Paper 702f:** Computational Study of Microscopic Drug Transport and Distribution in Tumor Vasculature — **Moath Alamer**, Xiao Yun Xu

**Paper 190aj:** High-Temporal-Resolution Measurements of Polymer Micellization Kinetics By Integrating a Microfluidic Device with Synchrotron X-Ray — **Joseph Kalkowski**, **Chang Liu**, Paola Leon Plata, Magdalena Szymusiak, Pin Zhang

**Paper 190ak:** Spatial-Temporal Dynamics of the Biofilm Formation — **Liliana Angeles-Martinez**, Vassily Hatzimanikatis

**Paper 190al:** Not Always Resistant: Antibiotic Susceptibility of Bacterial Cells Changes during Early Stage Biofilm Formation — **Huan Gu**, **Zhaowei Jiang**, **Dacheng Ren**

**Paper 190am:** Modulation of Ultrasensitive Signaling in Bacteria By Mechanical Forces — **Jyot Antani**, **Pushkar Lele**

**Paper 190ao:** Hyper-Activation of Cellular Rigidity Sensing By Solid Surface Tension of Biomaterials and Silicone Breast Implants — **Zhu Cheng**, Chung-Yuen Hui, Matthew Paszek

**Paper 190aq:** Dynamics and Mechanics of Rotational Collective Cell Movements — **Abraham E. Wolf**, **Celeste M. Nelson**

**Paper 190ar:** Modeling the Extensibility and Strain-Hardening Inelasticity of Fibrin Fibers during Coagulation — **Megan Cala**, Joseph J. McCarthy, Robert S. Parker

**Paper 190as:** Biophysical Model of CsrA-mRNA Interactions Expands Canonical Understanding of the CsrA Global Regulator Protein — **Abigail N. Leistra**, Grant Gelderman, Steven Sowa, Alex Moon-walker, Howard M. Salis, Lydia M. Contreras

**Paper 190at:** Detection of Truncation on RNA By RARE — **Wen-Jie Zhuang**, **Chung-Yu Wu**, **Chao-Lin Liu**

**Paper 190au:** Exploring Tumor Metabolic Heterogeneity through Integration of Single Cell RNA-Seq Analysis and Genome-Scale Metabolic Models — **Daniel Cook**, Jonathan L. Robinson, Jens Nielsen

**Paper 190av:** Using Metabolomics As a High-Sensitivity Quality Control Tool for the Characterization of Chondrogenic Microtissues — **Niki Loverdou**, Gabriella Nilsson Hall, Kristel Bernaerts, Bart Ghesquière, Geert Carmeliet, Ioannis Papantoniou, Liesbet Geris

**Paper 190aw:** Identifying an Individual's Comprehensive Epitope Repertoire — **Sumaiya Islam**, Robert Pantazes

**Paper 190ax:** Integrated Epigenome and Transcriptome Sequencing from the Same Cell — **Siddharth S. Dey**

**Paper 190ay:** CRISPR-Based Editing Reveals Edge-Specific Effects in Biological Networks — **Chance Nowak**

**Paper 190az:** Raps: Rapid Annotation of Photosynthetic Systems — **Alexander Metcalf**, **Nanette R. Boyle**

**Paper 190ba:** High-Throughput Screening of Alkaline Phosphatase Activity in Single Algal Cells Shows Heterogeneity Under Deviant Phosphorus Conditions — **Manibarathi Vaithyanathan**, Jacob Pettigrew, Travis Dugas, Yusef Kana, Ann Nguyen, Adam Melvin

**Paper 190bb:** Effect of Glycosylation on the Aggregation of Insulin Fragments — **Paul Praveen Nakka**, Daniel Forciniti

**Paper 190bc:** Synergistic Anti-Oxidation Effect of Resveratrol at Lipid Membrane Surface — **Jin Han**, Keishi Suga, Keita Hayashi, Yukihiko Okamoto, Hiroshi Umakoshi

**Paper 190bd:** Sucrose Concentration Determines Giant Unilamellar Vesicle Size during Electroformation — **Bridget Black**, Erica Spatafore, Gary Thompson

**Paper 190be:** Supported Biomembrane Microenvironments Characterized at the Micro- and Nanoscale for Gamma-Secretase Functional Analysis and Assays — **Lane Gilchrist**, William Houlihan, Marilia Barros, Eitan Wong, Yueming Li

**Paper 190bf:** Endocytosis and Trafficking of siRNA-Containing Complexes — **Daniel Vocelle**, Olivia Chesniak, Chauncey Splichal, Milton Smith, Christina Chan, S. Patrick Walton

**Paper 190bg:** Electrospun Microfibers and Lipid-Based Nanoparticles: A Combination Delivery System for Resveratrol and siRNA — **Thikrayat Al-Attar**, Sundararajan Madhally

**Paper 190bh:** Procaine Loading and Release from MIL-100 (Cr,Fe) and MIL-101(Cr,Fe), and Pectine-MOF Matrices — **Mehran Aliari Miavaghi**, **Banu Kocaaga**, **Ahmet Sirkecioglu**

**Paper 190bi:** Multiscale Structural Characterization of Epithelial Cell Monolayers Associated with the Addition of Permeability Enhancers for Enhancing Drug Delivery — **Shiyuan Zheng**, Katherine Fein, Nicholas G. Lamson, Kris Noel Dahl, Kirill Lavrenyuk, Kathryn Whitehead

**Paper 190bj:** Biophysical, Cytotoxicity and Cellular Uptake Studies of Novel Amphiphilic Fluorophores for Photodynamic Therapy (PDT) — **Poornima Kalyanram**, Istvan Stadler, Anju Gupta

**Paper 190bk:** Suprachoroidal Space Injection of in-Situ Forming Bevacizumab-Hyaluronic Acid Hydrogel Using a Microneedle to Increase Drug Retention Time — **Jae Hwan Jung**, Seongshik Kim, Mark R. Prausnitz



**Paper 190bm:** A Systems Engineering Framework for Diagnosis and Treatment of Chronic Obstructive Pulmonary Diseases (COPD) — **Navid Ghadipasha**, **Anais Chaland**, **Bin Yu**, **Babatunde A. Ogunnaik**

**Paper 190bn:** Network Motif Properties Influence Transmission of Autosomal Allelic Imbalance to Phenotype Relevant Signals — **Shibin Mathew**, **Alexander Gimelbrant**, **Suzanne Gaudet**

**Paper 190bo:** Genetic Engineering for the Production of Curcumin in Human Cells — **Logan Warriner**, **Daniel W. Pack**

**Paper 190bp:** Proteins Covalently Conjugated to Phenylpiperazine-Containing Polymers Experience Selectively Enhanced Intestinal Epithelial Transport — **Katherine Fein**, **Chad Cummings**, **Hironobu Murata**, **Rebecca Ball**, **Alan Russell**, **Kathryn A. Whitehead**

**Paper 190bq:** Spatial and Temporal Imaging Reveals Single-Cell Heterogeneity during Virus Growth and Infection Spread — **Huicheng Shi**, **John Yin**

**Paper 190br:** Blood Rheology across Species: Differences and Similarities — **Jeffrey S. Horner**, **Antony N. Beris**, **Norman J. Wagner**, **Donna S. Woulfe**

**Paper 190bs:** Addressing Complexity of Health Impact Assessment in Industrially Contaminated Sites Via the Exposome Paradigm — **Dimosthenis Sarigiannis**, **Spyros Karakitsios**

#### (191) Poster Session: Food and Bioprocess Engineering Monday, Oct 29, 3:30 PM

David L. Lawrence Convention Center, Exhibit Hall B

Michelle C. Almendrala, Chair  
Nutha Thongchul, Co-Chair

**Sponsored by:** Food

**Paper 191a:** Hybrid Mixture Theory-Based Modeling of Moisture Transport in Carrots during Drying — **Oguz Kaan Ozturk**, **Pawan Singh Takhar**

**Paper 191b:** Separation of Chitin from Shrimp Shells using Functional Ionic Liquids — **Xingmei Lyu**, **Mi Feng**, **Jie Zhang**, **Suojiang Zhang**

**Paper 191c:** Assessment of Oxidative Stability of Home-Cooked Meat Products in US By Targeted Lipidomics — **Lisaura Maldonado**

**Paper 191d:** Process Development for the Spray Drying of Milk Protein Stabilized Emulsions with High Oil Content — **Tonghan Gu**, **Laurie Brutus**, **Yinying Ren**, **Fan He**, **Angeliki A. Rigos**, **T. Alan Hatten**

**Paper 191e:** Linking Metabolizable Energy to Chemical Oxygen Demand — **Taylor L. Davis**, **Blake E. Dirks**, **Karen D. Corbin**, **Steven R. Smith**, **Bruce Rittmann**, **Rosy Krajmalnik-Brown**, **Andrew K. Marcus**

**Paper 191f:** An Experimental and Computational Study of Saponin Extraction — **Daniel Lepek**, **Jamie Chan**

**Paper 191g:** An Experimental and Computational Study of Saponin Extraction from Wine Grape Pomace — **Daniel Lepek**, **Jamie Chan**

**Paper 191h:** Comparison Data on Antioxidant Activities, Flavonoid and Mineral Content Analysis of *Artocarpus Altilis* Leaves at Different Maturity Stages — **Noorazwani Zainol**, **Norliza Abdul Latif**, **Siti Hajar Mat Sarip**, **Nor Farahiyah Aman Nor**, **Siti Alyani Mat**, **Norasiah Sadek**, **Harisun Yaakob**

**Paper 191i:** Influence of Chemical Structure of Compounds Present in Essential Oils on Their Antimicrobial Activity — **Ivan Horacio Rosano-Gazca**, **Nelly Ramirez-Corona**, **Aurelio López-Malo**, **María Teresa Jiménez-Munguía**, **Enrique Palou**

**Paper 191j:** Producing a Value Added Artificial Sweetener from Dairy Processing By-Product Via the Hydrogenation of Lactose — **Andrew Kasick**, **Sunggyu Lee**

**Paper 191k:** Physicochemical Properties, Macro- and Microanalytes Analysis of Gluten-Free Flour As Potential Functional Food Ingredients — **Noorazwani Zainol**, **Daneshwary Muniandi**, **Suhir Sulaiman**, **Siti Alyani Mat**, **Norasiah Sadek**, **Ramlan Aziz**

**Paper 191l:** Isosteviol: Synthesis through Typical Lewis Acid-Catalysis ( $\text{Fe}^{3+}$ ) and Preparation Thereof Inclusion Complex with  $\beta$ -CD — **Hui-da Wan**

**Paper 191m:** Raspberry-Derived Treatment of Inflammatory Bowel Disease — **Kyle E. Cochran**, **Nicholas G. Lamson**, **Kathryn A. Whitehead**

**Paper 191n:** Study of the Drying Kinetics of Sugar Cane Molasses Via Single Droplet Drying Technique — **Valeria D. Benalcázar**, **Paulo C. Narvaez**, **Alvaro Orjuela**

**Paper 191o:** Optimization of Supercritical  $\text{CO}_2$  Extraction to Maintain the Ratio of  $\omega$ -6 and  $\omega$ -3 Fatty Acid from Hemp Oil — **Vibha Devi**, **Shabina Khanam**

**Paper 191p:** Improved Performance of Biomimetic Membrane Integrated with the Aquaporins Modified with *in-Vitro* Genetic Incorporation of *P*-propargyloxyphenylalanine — **Peilian Wei**, **Bingjia Zhuang**, **Daoyong Yu**, **Sharipova Aziza**, **Jin Cai**, **Lei Huang**, **Jiazhang Lian**, **Zhinan Xu**

**Paper 191r:** Phospholipid Bilayer Functionalized Membrane for Immobilized Enzymatic Catalysis — **Anju Tiwari**, **Saurav Datta**

**Paper 191t:** Concentration of Polyphenols from Blueberry Pomace Extract Using Nanofiltration — **Arijit Sengupta**, **Alexandru Avram**, **S. Ranil Wickramasinghe**

**Paper 191u:** Enzymatic Hydrolysis for Maximum Co-Products Production of Non-Noble Metal Catalyzed Alkaline Hydrogen Peroxide and Alkaline Pre-Extracted Woody Biomass — **Sandip Kumar Singh**, **David Hodge**

**Paper 191v:** Cloning and Expression of Heparinase Gene from *Raoultella* Nx-TZ-3-15 — **Yingzi Jiang**, **Wenli Liu**, **Liqing Zhao**, **S.T. Yang**

**Paper 191w:** Fast Growing Novel Isolate of Cyanobacteria As a Platform for the Production of Succinate — **Shinjinee Sengupta**

**Paper 191x:** Efficient Production of (Z)- $\alpha$ -Santalol with Multi-Pathway Engineering in *Saccharomyces Cerevisiae* — **Zhuwei Shi**, **Lei Huang**, **Jiazhang Lian**, **Jin Cai**, **Zhinan Xu**

**Paper 191y:** Functional Characterization of Soypeptides As Supplementary Diet and Their Effects on the Kinetics of Cell Growth of Probiotic Microorganisms — **Noorazwani Zainol**, **Chin Keat Ho**, **Roslinda Abd Malek**, **Siti Zulaiha Hanapi**, **Siti Alyani Mat**, **Mun Leong Wong**, **Chee Loong Teo**, **Twee Juan Wong**, **Ani Idris**, **Hesham Elenshasy**

**Paper 191z:** N-Butanol Production from Cotton Stalk Using Engineered *Clostridium Cellulovorans* — **Jing Li**, **Wenjie Hou**, **Teng Bao**, **Shang-Tian Yang**

**Paper 191aa:** Oxidation-Reduction Potential Controlled Microaeration for Fermentation of Lignocellulose Feedstock — **John Moore**, **Patrick Gilcrease**

**Paper 191ab:** Semi-Continuous Fermentation of Acetic Acid By Mutant of *Acetobacter Pasteurianus* — **Qing Liu**, **Hongli Yao**, **Xingjiang Li**, **Zhi Zheng**, **Shaotong Jiang**, **Xuefeng Wu**, **Shang-Tian Yang**, **Xiaojing Jia**

**Paper 191ac:** Effects of Artificial Electron Carriers on High-Efficient Butyric Acid Production through Co-Fermentation of Glucose and Acetate By *Clostridium Tyrobutyricum* — **Hongxin Fu**, **Jufang Wang**, **Shang-Tian Yang**

**Paper 191ad:** System Metabolic Engineering of *Clostridium Cellulovorans* Towards Consolidated Bioprocessing for *N*-Butanol Production from Cellulosic Biomass — **Teng Bao**, **Jingbo Zhao**, **Shang-Tian Yang**

**Paper 191ae:** Improving the Fermentation Performance of *Clostridium Acetobutylicum* ATCC 824 By Strengthening the VB1 Biosynthesis Pathway — **Jufang Wang**, **Hongxin Fu**, **Zhengping Liao**

**Paper 191af:** Production Improvement and a Novel Separation Method of Bacteriocin Y31 Produced By *Enterococcus Faecium* Y31 — **Wenli Liu**, **Lanwei Zhang**

**Paper 191ag:** Optimization of Pleuran Production By *Pleurotus Ostreatus* Using Batch and Fed-Batch Cultivation System — **Roslinda Abd Malek**, **Mohd Helmi Johari Masri**, **Solleh Ramli**, **Daniel Joe Dailin**, **Siti Zulaiha Hanapi**, **Hesham Ali El-Enshasy**

**Paper 191ah:** Extraction, Purification and Modification of Poly (3-hydroxybutyrate) Produced By the Fermentation of Fatty Acids with *Burkholderia Cepacia* B27 — **Andrés Ramos Sr.**, **Armando Espinosa**, **Ivan Cabeza Sr.**

**Paper 191ai:** Analysis and Design of Kinetic Controls of Fatty Acid Synthesis — **Alex Ruppe**, **Jerome M. Fox**

**Paper 191aj:** Rewiring *Yarrowia Lipolytica* Lipid Metabolism for the Production of Omega-3 Fatty Acid Using Alternative Substrates — **Difeng Gao**, **Spencer Smith**, **Michael Spagnuolo**, **Mark Blenner**

**Paper 191ak:** Exploiting the L-Lactate Biosynthetic Pathway in *Corynebacterium Glutamicum* for Heterologous Production of D-Lactate from Biomass-Derived Carbon Substrates — **Amit Kumar Jha**, **Zohal Wardak**, **Benjamin Nauroth**, **Ryan W Davis**, **Mary Bao Tran-Gyamfi**, **John M. Gladden**, **Arul Varman**



**Paper 191a:** Homologous Constitutive Expression of Halophilic and Acidophilic  $\beta$ -Glucosidases in Marine *Aspergillus Niger* Zjube-1 — **Li-Nian Cai**, Sheng-Nan Xu, Dong-Qiang Lin, Shan-Jing Yao

**Paper 191am:** Adaptive Evolution of Microalgae *Schizochytrium* Sp. Under High Salinity Stress to Alleviate Oxidative Damage and Improve Lipid Biosynthesis — **Xiao-Man Sun**, Lu-Jing Ren, He Huang

**Paper 191an:** Adapted Evolution and Biosensor-Based Screening for Robust Growth of *Pseudomonas Putida* on Corn Stover Hydrolysate and *Cis*, *Cis*-Muconic Acid Production — **Niju Narayanan**, Scott Patrick Henelly, Christopher Johnson, Gregg T. Beckham, Taraka Dale, Ramesh Kumar Jha

**Paper 191ap:** A High-Throughput Platform Technology for Engineering Enhanced-Solubility in Biotherapeutics — **Andrew Chang**, Jacob Furlon, Karl E. Griswold

**Paper 191ar:** Well-Mixed Cancer-on-Chip System for the Simultaneous Evaluation of Toxicity and Efficacy of Anti-Cancer Drugs — **Everardo Gonzalez Gonzalez**, Grissel Trujillo-de Santiago, Salvador Gallegos Martinez, Abril Valverde Rascón, Ingrid Anaya Morales, Aimé A. Cuéllar Monterrubio, Andrés García Rubio, Brenda Flores García, Christian Mendoza Buenrostro, Ciro Angel Rodríguez-González, Augusto Rojas Martínez, Rocío Ortiz López, Mario Moisés Alvarez

**Paper 191as:** Modeling Chemical Transport in PDMS-Based Organ-on-Chip Microsystems — **Kazi Tasneem**, Alexander Auner, Dmitry Markov, Lisa McCawley, M. Shane Hutson

#### (192) Poster Session: Interfacial Phenomena (Area 1C)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Marina Tsianou, Chair  
Raymond Tu, Co-Chair

**Sponsored by:** Interfacial Phenomena

**Paper 192a:** Modeling of Fluid Transfer in Nanoporous Carbons with Molecular Dynamics Simulation — **Shanshan Wang**, Linghong Lu

**Paper 192b:** Study of Interfacial Modulus and Sliding Drop Motion By Centrifugal Adhesion Balance (CAB) — **Akash Jena**, Sirui Tang, Semih Gulec, Sakshi Yadav, Rafael Tadmor

**Paper 192c:** Impact of Dispersion Stability on Asphaltenes in Bulk and at Oil-Water Interfaces — **Junchi Ma**, Lynn M. Walker

**Paper 192d:** Atomistic Simulations of the Superlubricity between Graphene Nanoribbons and Au/Ag/Cu Surfaces — **Nariman Piroozan**, Muhammad Sahimi

**Paper 192e:** Responsiveness of Multi-Responsive Weak Polyelectrolyte Brush Grafted Nanoparticles with Varying Brush Characteristics — **Danish Iqbal**, Jiajun Yan, Robert D. Tilton, Krzysztof Matyjaszewski

**Paper 192f:** Mechanistic Study of Enzyme Immobilization on Flexible Tubing Surfaces — **Mahbuba Jannat**

**Paper 192g:** Electroemulsification and Purification of Water-in-Fuel Emulsions — **Ted J. Amundsen**, Andrew L. Wagner

**Paper 192h:** Dynamic Interactions between Oil Droplet and Oil Film in Complex Aqueous Environment — **Yumo Wang**, Wei Wang, Yun Shen, Yuntong Ge

**Paper 192i:** Effect of Non-Newtonian Bio-Transport Modeling on Vessel Concentration Predictions — **Elyse C. Tighe**, Steffano Oyanader, Mario Oyanader

**Paper 192j:** Modelling of Vessel Molar Transport Under Mural Electrical Field Gradient — **Jillian G. Arnold**, Chloe P. Winter, Mathias A. Oyanader, Mario Oyanader

**Paper 192k:** Fundamental Study of the Electrical Field Role in Drug Delivery — **Jewel C. Esparza**, Mathias A. Oyanader, Mario Oyanader, Steffano Oyanader

**Paper 192l:** Analysis of a 2D Ionophoretic System Using an Area Averaging Approach — **Alisa J. Kidwell**, Mario Oyanader, Steffano Oyanader

**Paper 192m:** Application of the Extended Correction Function Method to Solve the Poisson Boltzmann Equation Under Non-Isothermal Conditions — **QingQuan Xia**, Mario Oyanader

**Paper 192n:** Experimental and Theoretical Study on Supported Nanocatalysts — **Jianguo Wang**

**Paper 192o:** Role of  $C_3N_4$  and Pd in Selective Hydrogenation of Phenol — **Guangyu He Sr.**, Yingchun Liu

**Paper 192p:** Bridging Bulk and Interfacial Rheology of Clinical Lung Surfactants — **Clara O. Ciutara**, Joseph A. Zasadzinski

**Paper 192q:** Investigating Phase Fractions of DPPC-Hexadecanol Monolayers Using Fluorescence Microscopy of Langmuir Films — **Mitchell Kohler**, Cain Valtierrez-Gaytan, Ian Williams, Todd M. Squires, Joseph A. Zasadzinski

**Paper 192r:** Box-Behnken Design of Self-Emulsifying Emulsions for Application as Vaccine Adjuvants — **Yulia Burakova**, Jishu N. Shi, John R. Schlup

#### (193) Poster Session: Materials Engineering & Sciences (08A - Polymers)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Jeffrey Rimer, Chair  
Pinar Akcora, Co-Chair  
Julianne L. Holloway, Co-Chair

**Sponsored by:** Materials Engineering and Sciences Division

**Paper 193a:** Transfer Printing of Organic-Inorganic Multilayer Thin Films — **Soyoun Kim**, Nan Liu, Alexander Shestopalov

**Paper 193b:** The Effect of Crystallization and Glass Transition Temperature in Thin Poly(D,L-lactic acid) Copolymers for Controlling Osteoblast Recruitment and Adhesion — **Ufuoma Ikoba**, Nathan Gallant, Ryan Toomey

**Paper 193c:** Synthesis of a Chemically Protective, Moisture-Vapor Permeable Polymeric Membrane for Use in Protective Equipment — **James Ogilvie-Battersby**, Nese Orbey, Natalie Pomerantz, June Lum, Erin Anderson, Quoc Truong

**Paper 193d:** Heat Transfer across Tip-Surface Nanointerface: A Quantitative Model By Scanning Thermal Microscopy (SThM) — **Yifan Li**, Jiahua Zhu, Nitin Mehra

**Paper 193e:** Star Polymer-Assembled Thin Film Composite Membranes with High Separation Performance and Low Fouling — **Jung-Hyun Lee**

**Paper 193f:** Effect of Large Deformation on the Physical Age of Polymer Investigated By MultiStep Nonlinear Creep — **Yelin Ni**, Grigori A. Medvedev, James M. Caruthers

**Paper 193g:** In-Situ Investigation of Shear-Induced Close-Packed Spherical Morphology in an ABA Triblock Copolymer — **Wenyue Ding**, Shu Wang, Sameer Vajjala Kesava, Enrique D. Gomez, Wesley R. Burghardt, Megan L. Robertson

**Paper 193h:** Carbon Nanofiber Formation from Supercritical Carbon Dioxide Extraction Tar/PAN Via Electrospinning — **Xin He**, Maohong Fan

**Paper 193i:** Computational Fluid Dynamics Simulation of the Fused Deposition Modeling Process Using a Viscoelastic Model — **Behrouz Behdani**, Leah Mason, Ming Leu, Fateme Rezaei, Ali Rownaghi, Joontaek Park

**Paper 193j:** Adjusting the Mechanical Properties of Polypropylene By Long Chain Branching Molecular Structure Designing — **Shuai Zhou**, Zhong Xin

**Paper 193k:** Toughening of Triblock Copolymer Anion Exchange Membranes — **Onur Ozcalik**

**Paper 193l:** High Production Rate of Nafion Nanofibers Via needleless Electrospinning — **Monica Hwang**, Muizz Karenson, Yossef A. Elabd

**Paper 193m:** Modeling Electric Double Layer Formation and Strain Induced By a Single-Ion Conducting Polymer on a Two-Dimensional Crystal — **Aaron Woepfel**, Susan Fullerton-Shirey

**Paper 193bh:** Elucidating How Interactions between Functionalized Nanoparticles and Nafion Alter the Dispersion State and Vanadium Ion Permeability in Ionomer Nanocomposite Membranes — **Allison Jansto**, Eric M. Davis

**Paper 193n:** Flash Nanocomplexation: A Continuous and Scalable Platform for Functional Polyelectrolyte Complex Colloids — **Douglas Scott**, Robert K. Prud'homme, Rodney D. Priestley

**Paper 193o:** Effect of Salts on Material Properties and Responsive Behavior of Interpenetrating Polymer Network Hydrogels — **Philip Sitterle**, Yifei Xu, Lenore L. Dai

**Paper 193p:** Experimental and Macroscopic-Level Mechanistic Modeling Study of Self-Initiated High-Temperature Polymerization of Ethyl Acrylate — **Saeed Laki**, Ahmad Arabi Shamsabadi, Michael C. Grady, Andrew M. Rappe, Masoud Soroush

**Paper 193q:** Hydrophobic Surface Significantly Alters the Conformational Equilibria of Polyglycine — **Apratim Bhattacharya**

**Paper 193r:** Characterization of Thermo-Responsive Polymer-Liquid Crystal Nonwovens — **Shani Levit**, Ratib Stwodah, Christina Tang, McKenna Gillard

**Paper 193s:** Thermal Ageing Performance of Polyolefins Under Different Temperatures — **Stacy Pesek**, Huang Wu, Sharon Wu, Huang Jessica, Lai Yuming, Hu Yushan

**Paper 193t:** Effect of Encapsulated Drug Molecules on Block Copolymer Micelle Self-Assembly — **Tyler J. Cooksey**, Xiuli Li, Louis Madsen, Megan L. Robertson

**Paper 193u:** Modeling of Bivariate Distributions of Polymer Properties: Speeding up Simulations By Using Parallel Computing and 2D Probability Generating Functions — **Esteban Pintos**, Cecilia Fortunatti, Mariano Asteasuain

**Paper 193v:** Effect of Freezing Polymerization in Poly(*N*-isopropylacrylamide)-Alginate Hydrogels Preparation on Its Mechanical Strength and Thermoresponsive Properties — **Daiki Inomoto**, Junichi Ida, Tatsushi Matsuyama

**Paper 193w:** Titanium Oxide Hydrates As Optically Versatile Species in Inorganic-Organic Hybrids — **Alex Balzer**, Natalie Stingelin

**Paper 193x:** Incorporating Information from MD Simulations into COSMO-RS Predictions for Polymers — **Nick Austin**

**Paper 193y:** Investigating the Impacts of Microdomain Morphology on Reverse Micelle Mobility within Organogels — **William Walker**, Kenneth Mineart

**Paper 193z:** CBN-Loaded PVC Nanofiber Membrane for Metal Cation Recovery — **Erwin Escobar**, Grace M. Nisola, Lawrence A. Limjoco, Rosemarie Ann I. Cuevas, Khino J. Parohinog, Rey Eliseo C. Torrejos, Francis Kirby B. Burnea, Jin Yong Lee, Seong-Poong Lee, Wook-Jin Chung

**Paper 193aa:** Controlling Surface Charge Generated By Contact Electrification — **Siowling Soh**

**Paper 193ab:** Selective Recovery of PGM from Secondary Sources Using Nanofiber Based on Molecularly Imprinted Polymer — **Lawrence A. Limjoco**, Grace M. Nisola, Hiluf Tekle Fissaha, Rosemarie Ann I. Cuevas, Erwin C. Escobar, Khino J. Parohinog, Wook-Jin Chung

**Paper 193ac:** Cellulose Dissolution Mechanisms in Tetrabutylphosphonium Hydroxide-Water Mixtures As Explored By Molecular Dynamics — **Brad Crawford**, Ahmed E. Ismail

**Paper 193ad:** Hybrid Organic Linkers for Enhanced Thermally Conductive and Optically Transparent Polymeric Material By Engineering Inter-Molecular Interactions — **Nitin Mehra**, Yifan Li, Jiahua Zhu

**Paper 193ae:** Flammability and Structural Characterization of PE/EVA Blends Containing Keratin and DNA As a Flame Retardant Combinations — **Saul Sanchez**, Eduardo Ramirez, Jorge Albite, Yuresis Nufiez, Rogelio Ramirez

**Paper 193ag:** Gas Transport in Poly(arylene ether sulfones) with Finely Tuned Microstructure and Morphology — **Tanner Corrado**, Joseph Aboki, Lukas Cepkauskas, Ruilan Guo

**Paper 193ah:** Highly Polar Polymers Based on Poly(1,3-dioxolane) for Membrane CO<sub>2</sub>/N<sub>2</sub> Separation — **Junyi Liu**, Ho Bum Park, Haiqing Lin

**Paper 193ai:** In Situ Generation of a Self-Dispersed  $\beta$ -Nucleating Agent with Increased Nucleation Efficiency in Isotactic Polypropylene — **Qin Wei**, Shicheng Zhao, Zhong Xin

**Paper 193aj:** Structure of Amphipathic Dendrons in Non-Polar Environments — **Yang Wang**, Karolina Kosakowska, Henry S. Ashbaugh, Scott Grayson

**Paper 193ak:** Enhancement of Water Vapor Barrier Properties of Biodegradable Poly(butylene adipate-co-terephthalate) Films with Highly Oriented Organomontmorillonite — **Jiaxu Li**, Lei Lai, Linbo Wu, Steven J. Severtson, Wen-Jun Wang

**Paper 193am:** Tuning Pitch in Self-Assembled Block Copolymers through Homopolymer Addition: Effect of Homopolymer Molecular Weight on Lamellae Roughness — **Jakin B. Delony**, Caleb Breaux, Peter Ludovice, Clifford L. Henderson

**Paper 193an:** Effective Mechanical and Electrical Connections between Stretchable and Flexible Electronics — **Kunal Mondal**, Steven Erlenbach, Siyuan Ma, Andrew Fassler, Jim Holbery, Michael D. Dickey

**Paper 193ao:** Photoactive Polymers for Anti-Infective Materials — **Bharadwaja Srimat Tirumala Peddinti**

**Paper 193ap:** Can Gas Discharge Plasma be Used to Modify Ultra High Molecular Weight Polyethylene Surfaces and Improve Acrylic Bone Cement Bonding? — **Panik Moradian**, Bianca Cruz, Nina Abramzon, Keith M. Forward

**Paper 193aq:** Novel Chromogenic Sensors Enabled By Multi-Stimuli-Responsive Shape Memory Polymers Possessing Unconventional All-Room-Temperature Shape Memory Effects — **Calen Leverant**, Peng Jiang

**Paper 193ar:** Thermal Response Epoxy Under High Rate Impact Loading Via Incorporation of Diels-Alder Substructures — **Jian Gao**

**Paper 573g:** Synthesis and Characterization of Ladder-like Polysilsesquioxanes for Hard Coating Films — **Seon Oh Hwang**, Ju Yeon Lee, Sang-Hee Park, Min Gyu Shin, Kevin Injoe Jung, Hyun Wook Jung, Jung-Hyun Lee

**Paper 193as:** Structural Dynamics of Strongly Segregated Block Copolymer Electrolytes — **Oluwagbenga Iyiola**, Onyekachi Oparaji, Alec Sandy, Suresh Narayanan, Subramanian Ramakrishnan, Daniel Hallinan Jr.

**Paper 193at:** Self-Healable Polyelectrolytes Multilayer Films through a Layer-By-Layer Assembly — **Maxwell Ware**, Adam Alturaiki, Ju-Won Jeon

**Paper 193au:** Aromatic-Doped Polycaprolactone with Tunable Degradation Behavior — **Yawei Sun**, Jinli Zhang, Wei Li

**Paper 193av:** Structural Dynamics of Strongly Segregated Block Co-polymer Electrolytes — **Oluwagbenga Iyiola**, Onyekachi Oparaji, Subramanian Ramakrishnan, Alec Sandy, Suresh Narayanan, Daniel Hallinan Jr.

**Paper 193ax:** Carbon-Molybdenum Oxide Composites Synthesized through CO<sub>2</sub> Conversion from Mxene (Mo<sub>2</sub>CT<sub>x</sub>) As Anode of Lithium Ion Battery — **Ayeong Byeon**, Christine Hatter, Jae Hyun Park, Won Yeong Choi, Chi Won Ahn, Yury Gogotsi, Jae W. Lee

**Paper 193ay:** Alkaline Fuel Cell Performance of Saturated *N*-Heterocyclic Cationic Multiblock Polymers — **Monica Hwang**, Carl L. Willis, Yossef A. Elabd

**Paper 193az:** Thermodynamic Modeling of Aqueous Multivalent Polyelectrolyte Systems with Polyelectrolyte NRTL Model — **Yuan Li**, Yue Yu, Chau-Chyun Chen

**Paper 193ba:** Thermally Stable Peraryl Phosphonium Ionic Liquids and Molten Salts: Thermodynamic and Thermophysical Properties — **Benjamin Siu**, Cody G. Cassity, Alexander Badini, James H. Davis Jr., Kevin N. West, Richard A. O'Brien, Mohammed Soltani

**Paper 193bb:** Formation/Dissolution of Silver Filaments through an Ionic Liquid-Polymer Electrolyte Composite — **Zhongmou Chao**, Garrison M. Crouch, Donghoon Han, David Go, Paul W. Bohn, Susan Fullerton-Shirey

**Paper 193bc:** Nearly Precise Ionomers Designed for Ion Transport — **Lu Yan**, Lauren Hoang, Karen I. Winey

**Paper 193be:** Advanced Ionic Polymers Inspired By Ionenenes and High-Performance Polymers — **Kathryn E. O'Harra**, Emily DeVries, Danielle Noll, Enrique M. Jackson, Jason E. Bara

**Paper 193bf:** Single-Step Synthesis of Novel Polyionic Liquids Having Antibacterial Activity and Showing  $\pi$ -Electron Mediated Selectivity in Separation of Aromatics — **Mohanad Kamaz**, Arijit Sengupta, Mahmood Jebur, Xianghong Qian, S. Ranil Wickramasinghe

**Paper 193bg:** Mechanism of Dissociation Kinetics in Polyelectrolyte Complex Micelles — **Hao Wu**, Jeffrey M. Ting, Olivia Werba, Matthew V. Tirrell

## (194) Poster Session: Materials Engineering & Sciences (08B - Biomaterials)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Jeffrey Rimer, Chair  
Adam Ekenseair, Co-Chair  
Julianne L. Holloway, Co-Chair

**Sponsored by:** Materials Engineering and Sciences Division

## ■ DNA, PROTEIN, AND PEPTIDE BIOMATERIALS AND DELIVERY

**Paper 194a:** Investigation of a Tunable Synthesis Method for Protein and Peptide-directed Nanoparticles for Catalytic Materials — **Abdollah Mosleh**, Robert R. Beitle, M. Hassan Beyzavi

**Paper 194b:** Simple and Accurate Method to Calculate Circular Dichroism Spectra of Peptides and Proteins in Molecular Dynamics Simulations — **Juan Liu**, Zewei Wang, Shiyi Wang, Carole Perry, Candan Tamerler, Hendrik Heinz

**Paper 194c:** Peptide Adsorption on Hydroxyapatite Surfaces and Implications on Shape and Mineralization: Impact of Sequence and Electrolyte pH — **Juan Liu**, Samuel Edmund Hoff, Chandrani Pramanik, Tariq Jamil, Sarah Kay VanOosten, Kyle Boone, Candan Tamerler, Hendrik Heinz



**Paper 194e:** Formulation of Peptide and Protein Therapeutics into Nanoparticles for Prolonged Activity and Improved Delivery — **Kurt D. Ristroph**, *Paradorn Rummaneeethorn, Robert K. Prud'homme*

**Paper 194f:** Growth Factor Binding Peptides in PEGDA Based Wound Dressings to Promote and Enhance Healing in Diabetic Ulcers — **Gabriel Righes**, *Erin Tsai, Abigail Jones, Andrea Jimenez-Vergara, Dany Munoz-Pinto*

**Paper 194g:** Permeation Analysis of Large Molecules to the Surface of Protein-Conjugates with High-Density Polymer Coats — **Bibifatima Kaupbayeva**, *Hironobu Murata, James Winsor, Amber Lucas, Jonathan Minden, Alan Russell*

**Paper 194h:** Molecular Interaction of DNA with Cysteamine- and Polylysine-Acetate Modified Gold Surfaces for Single Nucleobase Identification — **Lesli Mark**, *Michael Shirts, Will Medlin, Prashant Nagpal, Hendrik Heinz*

## ■ TISSUE REPAIR AND REGENERATION

**Paper 194i:** Mechanism of Osteocalcin Interactions with Hydroxyapatite Surfaces and Hydrogen Phosphate Precursors for Bone Mineralization — **Mahdi Tavakol**, *Samuel Edmund Hoff, Juan Liu, Hendrik Heinz*

**Paper 194j:** Synthesis and Characterization of PLLA-PEG-PLLA Triblock Copolymers As Biodegradable Thermoplastic Elastomers for Peripheral Nerve Repair — **Yang Hu**, *Robert Newman, Adam Ekensear*

**Paper 194k:** Modeling of Intervertebral Disc Tissue Exposed to Pulsed Electric Fields — **Steven Schwartz**, *Cailyn Rhoads, Gary Thompson*

**Paper 194l:** Osteoblast Adhesion and Proliferation on Multi-Functional Polyampholyte Hydrogels with Covalently Attached Sibling Proteins — **Stephanie Haag**, *Matthew T Bernards*

## ■ ANTIFOULING AND ANTIMICROBIAL BIOMATERIALS

**Paper 194n:** Deposition of Anti-Fouling Materials Via Self-Polymerization of Small Molecules — **Wei-Bor Tsai**

**Paper 194o:** Bio-Ionic Liquid Conjugated Hydrogels As Highly Adhesive, Antimicrobial and Hemostatic Surgical Sealant for Traumatic Injury — **Vaishali Krishnadosh**, *Leah Filardi, Ethan Ellis, Andrew Kapetanakis, Nicole Rosselli, Jamie Shirts, Tyler Hannah, Caleb Miller, Akshar Patel, Iman Noshadi*

**Paper 194q:** Engineering an Adhesive and Antimicrobial Nanocomposite Hydrogel for Wound Healing Applications — **Brijesh Hirani, Ebrahim Mostafavi**, *Nasim Annabi*

**Paper 194r:** An Antimicrobial and Osteoinductive Adhesive for Treatment of Pre-Implant Diseases — **Ehsan Shirzaei Sani**, *Roberto Portillo Lara, Zahra Aldawood, Seyed Hossein Bassiri, Giuseppe Intini, Nasim Annabi*

## ■ DRUG DESIGN AND DELIVERY

**Paper 194s:** Sizing Drug Delivery Particles in Blood Plasma — **Aida Lopez-Ruiz, Mark Bannon**, *Zahra Wallizadeh, Kourtney Gans, Miriam Marquez, Kathleen McEnnis*

**Paper 194t:** Folate-Conjugated Negatively Charged Ternary Polyplexes for Targeted Gene Delivery — **Landon A. Mott**, *Caleb Akers, Daniel W. Pack*

**Paper 194u:** Extensive Intracellular Delivery Via Non-Charged Sequence-Defined Cell-Penetrating Oligomers — **Ngoc Phan**, *Christopher A. Alabi*

**Paper 194v:** Multi-Drug Loaded PLGA Microparticles for Cancer Treatment — **Amber C. Jerke**, *Jordan A. Hoops, Lily Cutler, Timothy M. Brenza*

**Paper 194w:** Antibody Dual-Conjugate Delivery for Endosomal Escape of siRNA — **Dana N. Thornlow**, *Christopher A. Alabi*

**Paper 194x:** Combination Nanoadjuvants for Influenza Vaccines — **Kathleen Ross**, *Sujata Senapati, Jessica Alley, David Verhoeven, Michael J. Wannemuehler, Marian Kohut, Surya Mallapragada, Balaji Narasimhan*

**Paper 194z:** Fluorescent Tagging of Interleukin-4 for Visualizing in-Vivo Release from Coated Implantable Polypropylene Mesh for Correlation of Release Patterns to Downstream Outcomes — **Alexis Nolfi**, *Daniel Hachim, Aimon Iftikhar, Bryan Brown*

**Paper 194aa:** Resveratrol Loaded Scaffolds Protect Mice Against Diet Induced Obesity and Glucose Intolerance — **Michael Hendley**, *Prakasam Annamalai, Michael Gower*

## ■ GENERAL

**Paper 194ab:** Development of Low Cost Magnetic Adsorbents of Gum Karaya and Poly(N-isopropylacrylamide-co-acrylamide) to Remove Brilliant Green Dye from Aqueous Solution — **Anjali Goyal**, *Hemant Mittal, Saeed Alhassan*

**Paper 194ac:** Evaluation of Microparticles Designed to Modify Adipocyte Endocrine Function — **Christopher Isely**, *Prakasam Annamalai, Michael Gower*

**Paper 194ad:** Toroidal-Spiral Particles for Islet Encapsulation — **Paola Leon Plata**, *Maryam Zaroudi, Colin Foster, Ying Liu*

**Paper 194ae:** Macrophage Polarization on Microporous Scaffolds and ECM Secretion of Fibroblasts — **Kyung Jae Jeong**

**Paper 194ag:** Dopant-Free Hydrogels with Intrinsic Photoluminescent, Injectable and Biodegradable Properties — **Yung-Hao Tsou**, *Xiaoyang Xu*

**Paper 194ah:** Optimized Process to Produce Gelatin Methacryloyl (GelMA) — **Victor Hugo Sánchez Rodríguez**, *Sara Cristina Pedroza, Grissel Trujillo-de Santiago, Mario Moisés Alvarez*

## (195) Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Jeffrey Rimer, Chair  
Kumar Varoon Agrawal, Co-Chair  
Julianne L. Holloway, Co-Chair

**Sponsored by:** Materials Engineering and Sciences Division

**Paper 195a:** Dual Role of Surfactants Towards a Rational Design of Zeolite Catalysts — **Aseem Chawla**, *Rui Li, Rishabh Jain, R. John Clark, James Sutjianto, Jeremy Palmer, Javier García-Martínez, Jeffrey D. Rimer*

**Paper 195b:** Ion-Exchange of Zeolite Coatings Crystallized on Metal to Obtain Materials with Enhanced Water Sorption Capacity — **Cigdem Atalay-Oral**, *Melkon Tatlier*

**Paper 195c:** Oriented and Silica-Beta Zeolite Membranes for n-Butanol Recovery from Its Dilute Aqueous Solution — **Hongyu Guo**, *Xiufeng Liu, Baoquan Zhang*

**Paper 195d:** Novel In Situ Methods to Resolve the Complex Pathways of Zeolite Crystal Growth Towards the Optimization of Microporous Catalyst Synthesis — **Madhuresh K. Choudhary**, *Manjesh Kumar, Rishabh Jain, Jeffrey D. Rimer*

**Paper 195e:** Control of Oxide Ceramic Fiber Crystallinity, Grain Size and Morphology — **Chin-Shuo Kang**

**Paper 195f:** Self-Assembly of Chiral Nanostructures of Molybdenum Oxide — **Jinchen Fan**, *Yang Zhao, Nicholas Kotov*

**Paper 195g:** Glass-Ceramic As a Solid Electrolyte for Lithium-Ion Batteries — **Taiye Salami**

**Paper 195h:** Force Field for Molybdenum Disulfide to Compute Bulk and Interfacial Properties with Electrolytes and Biomacromolecules in High Accuracy — **Juan Liu**, *Jin Zeng, Zewei Wang, Jiajun Chen, James J. De Yoreo, Yu Huang, Hendrik Heinz*

**Paper 195i:** Designing Inhibitors of Mineral Scale: A New Platform Based on Cooperative Microfluidic Assays and in Situ Atomic Force Microscopy — **Ricardo D. Sosa**, *Xi Geng, Jeremy C. Palmer, Michael A. Reynolds, Jacinta C. Conrad, Jeffrey D. Rimer*

**Paper 195j:** Synthesis Carbide from Supercritical CO<sub>2</sub>-Ethanol Extraction Residues of Powder River Basin Coal — **Kaidi Sun**, *Xin He, Wenyang Lu, Mingchen Tang, Tongtong Wang, Maohong Fan*

**Paper 195k:** Application of Liquid Injection ALD Deposited Nickel Oxide to Fabricate Mim Diode for Rectenna-Based Heat Harvesters — **Xianglei Li**, *Patrick J. Pinhero*

**Paper 195l:** Metal-Organic Frameworks As Template Shells for Enhanced Cobalt Oxide Electrocatalyst Performance — **Luke Huelsenbeck**, *Shelby Hooe, Arian Ghorbanpour, Gaurav Giri, Charles Machan*

**Paper 195m:** Structural Characterization of Defects in Hexagonal Boron Nitride Using Scanning Probe Spectroscopy — **Daichi Kozawa**, *Ananth Govind Rajan, Volodymyr Koman, Kevin Silmore, Pingwei Liu, Albert Tianxiang Liu, Daniel Blankschtein, Michael Strano*

## (196) Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Jeffrey Rimer, Chair  
Letian Dou, Co-Chair  
Julianne L. Holloway, Co-Chair

**Sponsored by:** Materials Engineering and Sciences Division

**Paper 196a:** Nanoporous Materials for Sub-Ambient Radiative Cooling — **Hannah Kim**, *Andrej Lenert*

**Paper 196b:** Lithium Ion Cathode Materials Prepared Using Glycerol As Solvent and Reactant — **Khaleel Hamad, Xing Yangchuan**

**Paper 196c:** All-Solid-State Li–Air Battery Based on Hollow Carbon Spheres Catalysts Derived from a Sol-Gel Route — **Yanghua He, Gang Wu**

**Paper 196d:** First-Principles Study of the Temperature Effect on Energy Gaps in High-Temperature Gas Sensor Materials — **Yuning Wu, Yuhua Duan, Paul R. Ohodnicki, Wissam A. Saidi, Benjamin T. Chorpene**

**Paper 196e:** Radiative Thermal Transport in Tunable Graphene-Based Hyperbolic Metamaterials — **Sean McSherry, Andrej Lenert**

**Paper 196f:** Design and Characteristics of Biodegradable and Implantable Batteries — **Harrison Hawkins, Leah Filardi, Meagan Schweiger, Ethan Ellis, Andy Kapetanakis, John Pletscher, Elizabeth Gutierrez, Alexis Lawless-Gattone, Iman Noshadi**

**Paper 196g:** Nanopattern Formation from Current-Driven Dynamics of Single-Layer Epitaxial Islands on Crystalline Conducting Substrates — **Ashish Kumar, Dwaipayan Dasgupta, Dimitrios Maroudas**

**Paper 196h:** Titanium Nitride Nanotube Arrays with Tunable Dimension/Sulfur Composite As Cathode Materials for Lithium Sulfur Battery with Improved Performance — **Wenduo Zeng, Zhao Wang, Mark Cheng, Simon Ng**

**Paper 196i:** Design Rules to Tailor the Localized Surface Plasmon Resonance Characteristic of Metal Oxide Nanocrystals — **Ankit Agrawal, Delia J. Milliron**

**Paper 196j:** Synthesis of Photoswitchable Quantum Dots for Superresolution Microscopy — **Kil Ho Lee, Abhilasha Dehankar, Abhijit Marar, Thomas Porter, Karine Thate, Carol Lynn Alpert, Peter Kner, Jessica O. Winter**

**Paper 196l:** Interface Engineering of Metal Oxynitride Heterostructures for Optoelectronic and Catalytic Applications — **Debtanu Maiti, Johnnie Cairns, John N. Kuhn, Venkat R. Bhethanabotla**

**Paper 196m:** Influence of Basis Set on the Electronic Structure and Physico-Chemical Properties of the Cerium Tribromide and the Cerium Trichloride: Two Lanthanide Compounds. — **Jean Baptiste Fankam Fankam**

## **(197) Poster Session: Materials Engineering & Sciences (08F – Composite Materials)**

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Jeffrey Rimer, Chair  
Jiahua Zhu, Co-Chair  
Julianne L. Holloway, Co-Chair

**Sponsored by:** Materials Engineering and Sciences Division

**Paper 197a:** Production of Three-Dimensional Porous Graphene for Sodium-Ion Batteries — **Annsley Mace, Melisa Montalvo, Ju-Won Jeon**

**Paper 197b:** Crown Ether-Decorated Phosphazene-Modified Magnetic Graphene Oxide As a Composite Adsorbent Material for Selective Lithium Ion Recovery from Seawater — **Khino J. Parohinog, Grace M. Nisola, Lawrence A. Limjuco, Hiluf Tekle Fissaha, Erwin C. Escobar, Seong-Poong Lee, Wook-Jin Chung**

**Paper 197d:** Thermo-Mechanical Properties of 3-D Printed Fiber Reinforced Nylon Composites — **Mahdi Mohammadzadeh, Ismail Fidan, Holly A. Stretz, Astrit Ameri**

**Paper 197f:** A Simple Synthesis Method of Thermoresponsive Polymer Immobilized Magnetite Nanoparticles for Heavy Metal Ions Recovery — **Kodai Hayashi, Junichi Ida, Tatsushi Matsuyama**

**Paper 197g:** Controlled Topology Toughening Epoxy Via Incorporation of Partially Reacted Substructures — **Jian Gao**

**Paper 197h:** Noble Gas Infused Neoprene Closed Cell Foams for Ultra-Low Thermal Conductivity Textiles — **Anton L. Cottrill, Jeffrey L. Moran, Jacopo Buongiorno, Michael Strano**

**Paper 197i:** Covalent Organic Framework Spheres, Hollow Fibers and Films with Pompon Structure — **Song Wang, Ziyang Zhang, Pingwei Liu, Wen-Jun Wang, Bo-Geng Li**

**Paper 197j:** Functionalized Porous Aromatic Frameworks for Rapid Boron Removal from Aqueous Solutions — **Jovan Kamcev, Mercedes Taylor, Jeffrey R. Long**

**Paper 197k:** Nanocomposite Ultra-Portable Sensor for on-Site Copper Detection in Potable Water — **Yang Lu, Guoqiang Yu, Xin Wei, Ju-Won Jeon, Zhanhu Guo, Evan K. Wujcik**

**Paper 197l:** Analysis of Structure-Property Relationships Via Finite Element Method to Predict Composite Mechanical Properties and a Comparison of Homogenization Techniques — **Joshua Arp, Mingzhe Jiang, Christopher L. Kitchens, Joseph Geddes, Sez Atamturktur, Andrew Brown**

**Paper 197m:** The Nature and Gas Sorption Performance of Cu(I) Species in Cu(I)-Mfu-4l Metal-Organic Frameworks — **Mona H. Mohamed, Yahui Yang, Götz Vesper, Nathaniel L. Rosi**

**Paper 197n:** Computational Model of Defect Propagation Mechanisms in ZIF-8 — **Rebecca Han, Nina Tyminska, David S. Sholl, J.R. Schmidt**

**Paper 197o:** Non-Invasive Imaging of Distribution of Coarse Aggregate in Hardened States Concrete Using Advanced Gamma Ray Computed Tomography — **Omar J. Farid, Abbas Sultan, Weina Meng, Kamal Khayat, Muthanna H. Al-Dahhan**

## **(198) Poster Session: Nanoscale Science and Engineering**

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Reginald E. Rogers Jr., Chair  
Micah J. Green, Co-Chair  
Artemis A. Boghossian, Co-Chair

**Sponsored by:** Nanoscale Science and Engineering Forum

**Paper 283f:** Effects of CeO<sub>2</sub> in CuO-ZnO Catalyst for the Deep Purification of CO Derived from Olefins at the Ambient Temperature — **Jinhua Huang, Liping Ye, Meng Kong, Bingxing Yang**

**Paper 231d:** Selectivity Enhancement of Nanowire Gas Sensors Using Impedance Spectroscopy and Artificial Neural Network — **Mohamed Kilani, Xuecheng Yu, Evan Schaefer, Guangzhao Mao**

**Paper 198a:** Quality By Design in Nanomedicine: Application to a Microemulsion Delivery System — **Eric Lambert, Michele Herneisey, Emma Shychuck, Allison Kachel, James K. Drennen III, Jelena M. Janjic**

**Paper 198b:** Polymer Coated Gold-Ferric Oxide Superparamagnetic Nanoparticles for Theranostic Applications — **Muhammad Raisul Abedin, Sutapa Barua**

**Paper 198c:** Development of Steroid Biosensors Using Corona Phase Molecular Recognition and Translation to Physiological Biologging — **Michael A. Lee, Song Wang, Naveed Bakh, Freddy T. Nguyen, Michael Strano**

**Paper 198d:** Self-Assembly of Graphene/Noble Metal Nanotube Composite Electrodes for Fuel Cells and Supercapacitors — **Gabrielle Milanesa, Alexander Mitropoulos, Kamil Woronowicz, F. John Burpo, Enoch Nagelli**

**Paper 198e:** Adipose Tissue Stem Cells Bioengineered in Nano-Biomimetic Col Scaffolds for Skin Tissue Engineering — **Abolfazl Akbarzadeh, Azizeh Rahmani Del Bakhshayesh, Effat Alizadeh, Soodabeh Davaran**

**Paper 198f:** Self-Assembly of 3D Graphene/Carbon Nanotube Electrodes Via Poly(acrylic) Acid/Nickel Complexing for Biosensor Applications — **An Vu, Kamil Woronowicz, Alexander Mitropoulos, F. John Burpo, Enoch Nagelli**

**Paper 198g:** 3D Carbon Nanomaterial/Platinum Microtube Composites for Oxygen Reduction Reaction Electrocatalysis in Fuel Cells — **Delaney Marbach, F. John Burpo, Enoch Nagelli**

**Paper 198h:** Size-Controlled Silver Nanoparticle Synthesis in a Jet-Mixing Reactor — **Pinaki Ranadive, Aamena Parulkar, Nicholas Brunelli**

**Paper 198i:** Mapping Evanescent Wave Scattering from Anisotropic Particles — **Aidin Rashidi, Christopher L. Wirth**

**Paper 198j:** The Synthesis of Monodisperse, Supported Nanoparticle Catalysts with Switchable Surfactants and the Effects of Calcination on Nanoparticle Characteristics — **Kristin Bryant, Steven R. Saunders**

**Paper 198l:** Proximal Interactions in Graphene-Magnetic Nanoparticle Interfacial Composites — **Abhilasha Dehankar, Ethel Perez-Hoyos, Jinsong Xu, Joshua Goldberger, Roland Kawakami, Ezekiel Johnston-Halperin, Jessica O. Winter**

**Paper 198m:** Probing the Kinetics of DNA-Surfactant Exchange Reactions for Carbon Nanotubes — **Niyousha Mohammadshafie, Fjorela Xhyliu, Geyou Ao**



**4:45 Paper 230f:** Numerical Investigation of Erosive Strength of Collapsing Cavitating Bubble in Cryogenic Environment Near Rigid Wall — **Arpit Mishra, Joydip Mondal, Arnab Roy, Rajaram Lakkaraju, Parthasarathi Ghosh**

**5:00 Paper 230g:** Postulation for a Novel Passive System for Post-Accident Reactor Containment Cooling — **Sudipta Pramanik, Kush Kumar Dewangan, Prasanta Kumar Das**

**5:15 Paper 230h:** Effect of Multiport Vapor Injection on the Performance of a GOX-LOX Direct Contact Condenser — **Jayachandran K N, Arnab Roy, Parthasarathi Ghosh**

**5:30 Paper 230i:** A Time-Space Adaptive Mesh Refinement Strategy for the Inverse Estimation of Transient Local Heat Flux — **Qing-Qing Yang, Jiu Luo, Yi Heng, Hao-Ran Lu, Dong-Chuan Mo, Shu-Shen Lyu**

**5:45 Paper 230j:** Mechanism and Kinetic of Moisture-Curing Process of Reactive Polyurethane Hot Melt Adhesive — **Li Sun, Zegang Zong, Weilan Xue, Xuoxiang Zeng**

### (231) Micro and Nanofabricated Sensors

**Monday, Oct 29, 3:30 PM**  
Westin Convention Center,  
Pennsylvania West

Evan K. Wujcik, Chair  
Kevin J. Cash, Co-Chair  
Dongmei (Katie) Li, Co-Chair

**Sponsored by:** Sensors

**3:30 Paper 231a:** Invited: Nano-Structured Materials Enabled High-Temperature Gas Sensors: From Resistor-Type Sensors to Passive SAW Sensors — **Yu Lei**

**4:02 Paper 231b:** Invited: Microprobe for Sensing of Multiple Neurochemicals *In Vivo* — **Harold G. Monbouquette**

**4:34 Paper 231c:** Enzyme-Conjugated Nanosensors with a Tunable Detection Limits for Small Bio-Molecule Monitoring — **Mark S. Ferris, Makayla K. Elms, Kevin J. Cash**

**4:51 Paper 231e:** Array of Nanostructured Electrode Tailored from Isolated to Continuum Monolayer for Chemical Sensing at Sub Parts per Trillion — **Jennifer A. Arcila, Rahul Tevatia, Ravi Saraf**

**5:08 Paper 231f:** A Living Transistor of Quasi-1D Metal Nanoparticle Arrays As a Platform to Study Cellular Activity — **Abhijeet Prasad, Ravi Saraf**

**5:25 Paper 231g:** Developing High Performance Low Cost Ammonia Sensors Based on a Substrate-Directed Solution Crystallization Process — **Xuecheng Yu, Mohamed Kilani, Evan Schaefer, Guangzhao Mao**

**5:42 Paper 231h:** Portable and Low-Cost Potentiostat System for Quantification of Cadmium in Wastewaters — **Christian Camilo Segura, Ana Lucía Campaña Perilla, Sergio Leonardo Flórez González, Mabel Juliana Noguera Contreras, Juan C Cruz, Johann F Osma**

### (232) Nanomaterial Applications for Human Health and the Environment

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center,  
310

Nastassja Lewinski, Co-Chair  
Yinlun Huang, Co-Chair

**Sponsored by:** General

**3:30 Paper 232a:** Super-Susceptible Magnetic Nanocrystal Clusters for Medicine and Environment Applications — **Qingbo Zhang, Zhen Xiao, Shen Tong, Linlin Zhang, Gang Bao, Vicki Colvin**

**3:48 Paper 232b:** Material Property Targets for Nanostructured Adsorptive Membranes in Residential Water Purification Applications — **Elvis Eugene, William A. Phillip, Alexander W. Dowling**

**4:06 Paper 232h:** Nanomagnetic Illuminators for *In Vivo* Optical Imaging of Osteoarthritic Knee Joints — **Mythreyi Unni, Brittany Partain, Kyle Allen, Carlos Rinaldi**

**4:24 Paper 232d:** pH Responsive Nanoparticle Films for Biofilm Microenvironment Evaluation — **Padryk Merkl, Georgios A. Sotiriou**

**4:42 Paper 232e:** Development and Use of Modeling Techniques and Continuous Biomolecule Detection Towards Diabetes Treatment — **Naveed Bakh, Gili Bisker, Michael A. Lee, Freddy T. Nguyen, Xun Gong, Daniel P. Salem, Michael Strano**

**5:00 Paper 232f:** Optical Nanosensors for Monitoring 3D Oxygen Gradients in *Pseudomonas Aeruginosa* Biofilms — **Megan Jewell, Anne Galyean, Kevin J. Cash**

**5:18 Paper 232g:** A Colorimetric Plasmonic Nanosensor Hydrogel for the Detection of Spatial Dose Deposition of Ionizing Radiation for Clinical Radiotherapy — **Karthik Pushpavanam, Sahil Inamdar, Tomasz Bista, Eric Boshoven, Stephen Sapareto, Kaushal Rege**

**5:36 Paper 232c:** Electrospray-Mediated Flash Nanoprecipitation for Synthesizing Drug Delivery Nanocarriers — **Kil Ho Lee, Lauren Cosby, Atefeh Alizadehbirjandi, Barbara E. Wyslouzil, Jessica O. Winter**

### (233) Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center,  
412

Doh Change Lee, Chair

**Sponsored by:** Nanomaterials for Applications in Energy and Biology

**3:30 Paper 233a:** Unusual Electronic Properties of Template-Directed  $\pi$ -Conjugated Porphyrin and Phosphorene Nanotubes — **Bryan M. Wong, Sarah I. Allec, Niranjana V. Ilawale**

**3:50 Paper 233b:** Modeling the Aggregation Behavior of Cyanine Dyes for Efficient Energy Transport — **William P. Bricker, James L. Banal, Matthew B. Stone, Wei Jia Chen, Gabriela S. Schlau-Cohen, Mark Bathe**

**4:10 Paper 233c:** Spatial Tailoring of Dopant Position in Solids for Enhanced Visible Light Photocatalytic Performance — **Pragathi Darapaneni, Natalia da Silva Moura, James Dorman**

**4:30 Paper 233d:** Enhancement of Photocatalytic Reduction Reaction on TiO<sub>2</sub> Under Solar Light Using Alternative Plasmonic Titanium Nitride Nanoparticles — **Alyssa Beierle, Hanqing Pan, Michael D. Heagy, Sanchari Chowdhury**

**4:50 Paper 233e:** ZnO Nano Forest As Electrode Material for DSSC: Where Is the Bottleneck? — **Jayanta Chakraborty, Surajit Ghosh**

**5:10 Paper 233f:** Ultrathin Plasmonic Coatings for Selective Radiative Transmission in Silica Aerogels — **Zachary Berquist, Ashley R Bielinski, Hannah Kim, Neil P Dasgupta, Andrej Lenert**

### (234) New Developments in Computational Catalysis II

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center,  
402

Eric Walker, Chair  
Masoudeh Ahmadi, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 234a:** Modeling Heterogeneous Electrocatalysis on Realistic Surfaces from First-Principles, Thermodynamics, and Machine Learning — **Andrew M. Rappe**

**4:02 Paper 234b:** Uncovering Reaction Maps to Promote Active Catalysis — **Paul M. Zimmerman**

**4:20 Paper 234c:** Liquid Phase Modeling in Heterogeneous Catalysis — **Mohammad Saleheen, Andreas Heyden**

**4:38 Paper 234d:** Improving the Initial Guess for a Nudged Elastic Band Calculation By Incorporating Chemical Intuition — **Kyle Groden, Jean-Sabin McEwen**

**4:56 Paper 234e:** Improving the Efficiency of Kinetic Monte Carlo Simulations for Catalysis with a Parallel Caching Algorithm — **Michail Stamatakis**

**5:14 Paper 234f:** Machine Learning Molecular Dynamics for Understanding Nonadiabatic Surface Reactions — **Jiamin Wang, Hongliang Xin**

**5:32 Paper 234g:** Mapping the Degree of Rate Control Using Automated Construction of Microkinetic Models with Rmg-Cat — **Emily Mazeau, David Farina Jr., Richard H. West, Katrin Blondal, C. Franklin Goldsmith**

### (235) Novel Approaches to CO<sub>2</sub> Utilization

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center,  
321

Lynn Brickett, Chair  
Rameshwar D. Srivastava, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**3:30 Paper 235i:** The U.S. Department of Energy's R&D Program for Carbon Use and Reuse — **Lynn Brickett, John Litynski**

**3:45 Paper 235a:** Enabling a Solid-State Carbon Dioxide Distribution Network — **Kevin Blinn, Daniel Kopp, Jun Wang, Richard E. Riman**

**4:03 Paper 235b:** Plasma and Fluidic Oscillation Assisted Electrolysis of CO<sub>2</sub> — **Rachael H. Rothman, Ann V. Call, Tom Butterworth, Thomas Holmes, Lik Hang Hugo Tse, Pratik Desai, William B. Zimmerman**

**4:21 Paper 235c:** Treatment and Extraction of Metals from Electronic Wastes Using a Novel Solvent Containing Supercritical CO<sub>2</sub> — **Emily Hsu, Ah-Hyung Alissa Park, Alan C. West, Katayun Barmak**

**Paper 198n:** Characterizing the Aqueous Dispersion of DNA-Assisted Boron Nitride Nanotubes — **Venkateswara Rao Kode**, *Camerin McDonald, John Weicherding, Tony Dobrila, Petru S. Fodor, Christopher L. Wirth, Geyou Ao*

**Paper 198o:** Optimizing Design Parameters of a VLA-4-Targeted Liposomal Nanoparticle in a Multiple Myeloma Disease Model — **David Omstead**, *Basar Bilgicer*

**Paper 198p:** Evaluation of Mucus-Penetrating Nanocomposite Microparticles for Cystic Fibrosis-Related Infections — **Elisa A. Torrico Guzmán**, *Samantha A. Meenach*

**Paper 198q:** Nanoharvesting and Nanodelivery of Bioactive Materials Using Engineered Silica Nanoparticles — **M. Arif Khan**, *John M. Littleton, Stephen E. Rankin, Barbara L. Knutson*

**Paper 198s:** Nanoclustering of Salicylic Acid in Organic Solvents — **Shubhangi Kakkar**, *Renuka Devi Krishnaraj, Ake Rasmuson*

**Paper 198t:** Rapid Photo-Actuation of a DNA Nanostructure Using an Internal Photocaged Trigger Strand — **Nicholas Stephanopoulos**

**Paper 198u:** Targeted Delivery of a Drug Coupled Gold Nanoconjugate Induces Respiratory Recovery Following Cervical Spinal Cord Injury in Rats — **Fangchao Liu**, *Janelle Buttry, Zeljka Minic, Harry G. Goshgarian, Guangzhao Mao*

**Paper 198v:** The Implications of Competitive Adsorption on Lipoprotein-Nanoparticle Biodistribution — **Uche Anozie**, *Aaron M. Prescott, Steven M. Abel, Paul Dalhaimer*

**Paper 198w:** Development of Interfacial Mechanical Strength for Armored Gas Filled Capsules — **Charles Sharkey**, *Shelley L. Anna*

**Paper 198x:** A Colorimetric Sensor for the Detection and Quantification of Therapeutic Levels of Ionizing Radiation — **Karthik Pushpavanam**, *Sahil Inamdar, Subhadeep Dutta, Tomasz Bista, Eric Boshoven, Stephen Sapareto, Kaushal Rege*

**Paper 198y:** Probing Nanoclustering of Fenoxycarb in Isopropanol Solutions — **Renuka Devi Krishnaraj**, *Michael Svard, Dikshitkumar Khmar, Ake Rasmuson*

**Paper 198z:** Effects of Silica Nanoparticles in PVDF-SiO<sub>2</sub> Mixed Matrix Membranes Developed Via Immersion Precipitation Phase Inversion — **John Miles II**, *D. Bhattacharyya*

**Paper 198aa:** Carbon Black Morphology, Light Scattering and Direct Radiative Forcing — **Georgios A. Kelesidis**, *Mohammad Reza Kholghy, Joel Zuercher, Julian Robertz, Martin Allemann, Aleksandar Duric, Sotiris E. Pratsinis*

**Paper 198ab:** Chitosan Electrospun Nanofibers Functionalized with Collagen By Carboxamide Bond Formation — **Alejandra Perez-Nava**, *Mario Valle-Sanchez, Josué Mota-Morales, Luis Chacon-Garcia, Yliana Lopez-Castro, Judit Aviña-Verduzco, J. Betzabe González-Campos*

**Paper 198ac:** Electrospun Nanofibers from a Blend of Asphaltenes with Cellulose Acetate — **Efstathios Svinterikos**, *Mohamed Al Marzouqi, Ioannis Zuburtikudis*

**Paper 198ad:** Massive Enhancement of Optical Transmission across a Thin Metal Film Via Wave Vector Matching in Grating-Coupled Surface Plasmon Resonance — **Russell Mahmood**, *Michael B. Johnson, Andrew C. Hillier*

**Paper 198ae:** PVA-Based Nanostructured Catalysts Support Functionalized with Pyrrolylquinone-Tetrazole — **José Ismael Rangel-Ortiz**, *J. Betzabe González-Campos, Luis Chacon-Garcia*

**Paper 198af:** Investigations into the Generation of Chitin Nanofibers By Cryogenic Grinding — **Amy L. Lindenberger**, *Sunggyu Lee*

**Paper 198ag:** Study of ZIF-8 MOF's as Viable Drug Carriers — **David Ramirez-Ortega**, *Mariano Jimenez-Camus, Tomás-Eduardo Chávez-Miyauchi, Adriana Benítez-Rico, Marco-Antonio Loza-Mejía*

**Paper 198ah:** Can Nanotechnology Land a Solution for the Energy Security Challenge? — **Nouf AlJabri**, *Yun Chang, Kuo-Wei Huang*

**Paper 198aj:** Synthesis and Characterization of Biogenic Selenium Nanoparticles with Antibacterial Properties — **David Medina**, *Guijie Mi, Thomas J. Webster*

**Paper 198ak:** Nanoescapology Enabled By Surface-Engineered Magnetite: Novel Routes for Targeted Drug Delivery — **Natalia Lopez-Barbosa**, *Javier F Cifuentes, Carolina Muñoz Camargo, Andrés Fernando González-Barrios, Johann F Osma, Juan C Cruz*

**Paper 198al:** Novel Glucosylceramide Synthase Inhibitor Based Prodrug Copolymer Micelles for Delivery of Doxorubicin — **Jieni Xu**

**Paper 198am:** Influence of Micro and Nanoscale Surface Roughness on the Wetting Characteristics of Flat Surface — **Deepa Dixit**, *Chinmay Ghoroi*

**Paper 198an:** Synthesis and Characterization of Hollow Gold Nanoparticles for Gene Delivery — **Konstantin Mamedov**, *Anisha Veeren, JeongEun Shin, Sarah Merkel, Mark Osborn, Joseph A. Zasadzinski*

**(199) Poster Session: Novel Products from Forest and Plant Biomass**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

**Shri Ramaswamy**, Chair  
**Junyong Zhu**, Co-Chair

**Sponsored by:** Forest and Plant Bioproducts Division

**Paper 199a:** Synthesis and Potential Antiproliferative Activity of Dehydroabietylamine Imidazole Derivatives — **Fengyi Zhao**, *Li Xu, Wen Lu, Dong Jiang, Xu Sun, Shilong Yang, Feng Lin, Mengyi Zhou, Fuliang Cao*

**Paper 199b:** Protein Content and Amino Acids Profile in Ten Cultivars of Ginkgo (*Ginkgo biloba* L.) Nut from China — **Mengyi Zhou**, *Li Xu*

**Paper 199c:** Hydrothermal Treatment of Paper Mill Sludge: Nutrient Characterization — **Nepu Saha**, *M.Toufiq Reza*

**Paper 199d:** Inhibitory Effect of Biomass Hydrolysates on Glucose Transport in Microbial Fermentation — **Xin Tan**, *Maobing Tu*

**Paper 199e:** Effects of *P*-Hydroxybenzoic Acid and 2-Naphthol on Dilute Acid Pretreatment of Aspen — **Yequan Sheng**, *Maobing Tu*

**Paper 199f:** Investigating the Sorption Capacity of Hydrochar for Organic Pollutants and Comparing with That of Powdered Activated Carbon (PAC) As a Method of Treating Contaminated Water — **Huy Nguyen**, *Jeremy Taylor, Justinus A. Satrio*

**Paper 199g:** Synthesis of Hardwood Lignin Model Polymer and Its Effect on Enzymatic Hydrolysis of Cellulose — **Conghui Yue**, *Maobing Tu, Hairong Guan*

**Paper 199h:** Extraction and Recovery of Sinapic Acid from Oleaginous Biomass (Mustard Bran): A Sustainable Access to a Valuable Phenolic Platform Chemical — **Ezine Achinivu**, *Erika Clavijo Rivera, Amandine Flourat, Florent Allais*

**Paper 199i:** Process Design for Conversion of Coconut Coir Pith to Bioplastic and Byproducts — **Erin Haug**, *Felipe Reyes Gaibor, Alex Papadakis, Patricia Popescu, Huajiang Huang, Rengasamy Kasinathan, Bandaru V. Ramarao, Shri Ramaswamy*

**Paper 199k:** Selecting Solvents for Lignin Value Prior to Pulp — **Thomas T. Kwok**, *Christopher O. Luettgen, Matthew Realff, Andreas S. Bommarius*

**Paper 199l:** A Study on Extent of Chain Crosslink on HDT Improvement of Poly (lactic acid) — **Feng Wu**, *Amar K. Mohanty, Manju Misra*

**Paper 70c:** Effect of Lignin on Nanofibrillated Cellulose Production — **Qiang Yang**

**(200) Poster Session: Pharmaceutical**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

**Jonathan McMullen**, Chair  
**Christopher H. Marton**, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**Paper 200a:** Multi-Scale Modeling in Immuno-Oncology to Support Immunotherapy Drug Development — **Mohammad Ghasemi**, *Donald E. Mager*

**Paper 200b:** Evaluation of Microfluidic Device Designs for a Potassium Release Toxicity Assay — **Joseph Wakim**, *Nese Orbey, Carol Barry*

**Paper 200c:** Effects of Unsaturated Phospholipid Dilinoleoylphosphatidylcholine on Degradation of Phospholipid Vesicles Catalyzed By a Model Phospholipase A2 — **Pin Zhang**, *Veronica Villanueva, Joseph Kalkowski, Chang Liu, Tiep Hoang Pham, Wei Bu, Binhua Lin, Ying Liu*

**Paper 200d:** Peptoid JPT1A Reduces RAGE Expression and Attenuates Inflammatory Response: A Potential AD Therapeutic — **Lauren M. Wolf, Melissa A. Moss, Shannon L. Servoss**

**Paper 200e:** Rapid and Efficient Development of Downstream Bio-Pharmaceutical Processing Alternatives — **Giorgio Colombo, Isuru A. Udugama, Krist V. Gernaey, Seyed Soheil Mansouri**

**Paper 200f:** Pump-Down the Mycobacterium Tuberculosis: A DNA Gyrase/P-Glycoprotein Combined Inhibition Approach — **Erik Laurini, Suzana Aulic, Domenico Marson, Maurizio Fermeglia, Irene Briguglio, Roberta Ibba, Antonio Carta, Sabrina Pricl**

**Paper 200g:** Continuous Processing of Doxorubicin-Loaded Liposomes — **Antonio Costa, Raj Mukherjee, Anand Gupta, Gowtham Yenduri, Xiaoming Xu, Celia N. Cruz, Bodhisattwa Chaudhuri, Diane Burgess**

**Paper 200h:** Experiments and Multi-Scale Models to Understand Liposome Processing Using a Turbulent Jet in Co-Flow — **Raj Mukherjee, Antonio Costa, Anand Gupta, Gowtham Yenduri, Xiaoming Xu, Celia N. Cruz, Bodhisattwa Chaudhuri, Diane Burgess**

**Paper 200i:** Continuous Protein Crystallization of Lysozyme — **Huaiyu Yang, Wenqian Chen, Xiaoyu Li, Peter Peculis, Pavan Inguva, Jerry Y.Y. Heng**

**Paper 200j:** Development of a Cation Exchange Chromatography Step for Robust Impurity Clearance and Improved Polysorbate 80 Stability in the Drug Product of a Monoclonal Antibody — **Justin Miller, Rebecca A. Chmielowski, Seth Clark, Hong Li**

**Paper 200k:** Production of Anti-CD20 Monoclonal Antibody Biosimilar — **Jianfa Ou, Yingnan Si, Ningning Xu, Daniel D. Flanagan, Jiajia Song, Lufang Zhou, X. Margaret Liu**

**Paper 200l:** Multi-Stage and Multi-Objective Design Tool for Process Design in Sterile Filling of Biopharmaceuticals — **Haruku Shirahata, Philipp Zürcher, Sara Badr, Hirokazu Sugiyama**

**Paper 200m:** Comparison of Batch and Continuous Biopharmaceutical Antibody Production Based on Techno-Economic Analysis — **Ou Yang, Marianthi Ierapetritou**

**Paper 200n:** Increasing Capacity and Lifetime of Reverse Phase Resin — **William McKechnie, Sunitha Kandula, Nihal Tugcu**

**Paper 200o:** Liquid Phase Synthesis of Monodisperse PEGs By Nanostar Sieving — **Danilo Cuccato, Piers Gaffney, Ruiyi Liu, Marc Schaepertoens, Andrew G. Livingston**

**Paper 200p:** Virtual Screening of Process Parameters for Pharmaceutical Drying Operation: A Combined DoE-CFD Approach — **Deepak Jain, Joydeep Kant, Vishwanath Dalvi, Channamallikarjun Mathpati**

**Paper 200q:** Directed Cp\*Rh(III)-Catalyzed Fluorosulfonylvinilation of Arenes — **Gqwetha Ncube, Malcolm P. Huestis**

**Paper 200s:** Stoichiometry Identification in Pharmaceutical Reactions Using Dynamic Response Surface Methodology and Target Factor Analysis — **Yachao Dong, Christos Georgakis, Jacob Santos-Marques, Jason Mustakis, Ke Wang, Jonathan P. McMullen, Shane T. Grosser**

**Paper 200t:** Heat Transfer Transients in Semi-Batch Systems: A Computational Approach to Process Intensification and Mitigating Process Hazards — **Deepak Jain, Joydeep Kant, Vishwanath Dalvi, Channamallikarjun Mathpati**

**Paper 200u:** Plasmonic Nanocatalysts for Continuous Synthesis of Drug Substances: An Example of Visible-Light Mediated Cross Coupling Reactions — **Ravi Teja, Andishaeh Dadgar, Farshid Mohammadparast, Marimuthu Andiappan**

**Paper 200w:** Development and Scale-up of a Robust Impinging Jet Process Under GMP Conditions — **Anuj A. Verma, Kushal Sinha, Shashank Shekhar**

**Paper 200x:** Single-Step Continuous Purification from Liquid-Liquid-Solid Mixture: Design and Experimental Implementation for an HIV Drug Intermediate — **Mo Jiang, Boxuan Li, Amos E. Lu, Thomas D. Roper, Frank Gupton, Richard Braatz**

**Paper 200y:** Manipulation of Crystal Morphology of Zoxamide Based on Phase Diagram and Crystal Structure Analysis — **Hao Wu, Shuyi Zong, Qi Liu, Jingkang Wang, Hongxun Hao**

**Paper 200z:** Crystallization Kinetic Measurement and Parameter Estimation Utilizing Population Balance Model in a Dynamic/Oscillatory Baffle Crystallizer — **Claire Yiqing Liu, Ayse Eren, Paul Firth, Alastair Barton, Jonathon Speed, Dan Wood, Zoltan K. Nagy**

**Paper 200aa:** Nucleation Kinetics of Pharmaceutical Co-Crystals — **Hannah McTague**

**Paper 200ab:** Extrudability Analysis of Drug Loaded Pastes for 3D Printing of Modified Release Tablets — **Alaadin Alayoubi, Ahmed Zidan, James Coburn, Bahaa Ghamraoui, Celia N. Cruz, Muhammad Ashraf**

**Paper 200ac:** One Step Purification of Curcumin from Its Lower Grades Via Particle Mediated Crystallization — **Vasanth Kumar Kannuchamy, Kirankumar Ramisetty, Rama Krishna Gamidi, Claire Heffernan, Renuka Devi Krishnaraj, B. Kieran Hodnett, Ake Rasmuson**

**Paper 200ad:** Ternary Phase Diagram and Population Balance Model for Solvent-Mediated Phase Transformation of Lansoprazole — **Shuyi Zong, Hongxun Hao, Jingkang Wang, Hao Wu, Qi Liu**

**Paper 200ae:** Advancing Smart Manufacturing in Pharmaceutical Systems — **Sudarshan Ganesh, Mariana Moreno, Qinglin Su, Francesco Rossi, Marcial Gonzalez, Zoltan K. Nagy, G. V. Rex Reklaitis**

**Paper 200af:** Dropwise Manufacturing of Oral Solid Dosage Forms Using Powder Slurries — **Andrew J. Radcliffe, Zoltan K. Nagy, Gintaras V. Reklaitis**

**Paper 200ag:** Effect of Process Parameters on Stability of Lactate Dehydrogenase during Bulk Freeze-Thaw — **Bruna Minatovicz, Li Sun, Robin Bogner, Bodhisattwa Chaudhuri, Tai-Hsi Fan, Ji-Qin Li**

**Paper 200ah:** Effect of Solvent in Strip Film Manufacturing Containing BCS CLASS II Drugs VIA Solution Casting — **Eylul Cetindag, John Pentangelo, Rajesh Davé**

**Paper 200ai:** Droplet-Coalescence Kinetics for a Non-Newtonian Emulsion Using a Taylor-Couette Shear-Flow Reactor: Characterizing Phase-Separation Risk for a Pharmaceutical Ointment — **Arya Ketabchi-Haghighat, R. Dennis Vigil, Michael Olsen, Avik Sarkar**

**Paper 200aj:** Unique Polymorph and Amorphous Dispersion Formation of Suberic Acid Using Monodisperse Droplet Evaporation — **Victoria Karakis, Erin Dittmar, Kurt R. Vostal, Ryan C. Snyder**

**Paper 200ak:** Importance of the Reaction Kinetics of Drug-Bile Micelle Formation in Oral-Drug Absorption Modeling — **Brian Shoemaker, Fady Ibrahim, Ravi M. Shanker, Avik Sarkar**

**Paper 200al:** Anti-Static Agent Addition in Excipients – Always a Decent Way to Increase Powder Process-Ability in Pharmaceutical Industries? — **Quentin Ribeyre, Simon Bocquet, Filip Francqui, Geoffroy Lumay**

**Paper 200am:** CRISPR-Cas9 Plasmid DNA Delivery to Endometrial Cancer Cells for Knockout of PLAC1 — **Brittany E. Givens, Eric J. Devor, Aliasger K. Salem**

**Paper 200an:** Sustained Release Polymeric Drug Delivery Systems to Inhibit ERK1/2 Activity — **Brittany E. Givens, Youssef W. Naguib, Supreeda Tambunlerchai, Khanidtha Chitphet, Aliasger K. Salem**

**Paper 200ao:** Functionalized Ultra-Thin Shell Microcapsule for Targeted Encapsulation and Release — **Liyuan Zhang, Johnathan Didier, David A. Weitz**

## (201) Poster Session: Upstream Engineering and Flow Assurance

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

Mohammad Tavakkoli, Chair  
Francisco Vargas, Co-Chair  
Sandeep Verma, Co-Chair  
Michael P. Hoepfner, Co-Chair  
Sandhya Sundar Ram, Co-Chair  
Vikram Subramani, Co-Chair

**Sponsored by:** Upstream Engineering and Flow Assurance Forum

## ■ UPSTREAM ENGINEERING AND FLOW ASSURANCE

**Paper 201a:** Hydrate Risk Management during Cold Restart Operation Using MEG and Khi — **Yutaek Seo, Ki Heum Park**

**Paper 201b:** A Microfluidics Based Study on the Effect of Immiscible Huff-n-Puff Process on Residual Oil Saturation in Hydrophilic and Hydrophobic Porous Media — **Sushobhan Pradhan, Gbue Kone, Ryan Antle, Clint Aichele, Haifeng Jiang, Prem Bikina**

**Paper 201c:** Estimating the Drainage Area of Frac-HIT or RE-Fractured Horizontal Well — **Nitish Goyal, Matteo Marongiu-Porcu, Michael Nikolaou**

**Paper 201d:** Multiphase Flowloop Investigation of Transportability and Flow Properties of Highly Concentrated Hydrate Slurries — **Ben Bbosa, Michael Volk**

**Paper 201e:** Mitigation of Severe Slugging with Internal Model Control — **Ki Heum Park, Yutaek Seo, Jakyung Kim**



**Paper 2011f:** Investigation of the Interaction between Wax Precipitation and Hydrate Formation in Water-in-Oil (W/O) Emulsions — **Yuchuan Chen, Bohui Shi, Yang Liu, Jing Gong**

**Paper 201g:** Electrical Treatment of Waxy Crude Oil to Address Wax-Related Flow Assurance Issues — **Yingda Lu, Jinjun Zhang, Chenbo Ma, Chaohui Chen, Xinyi Wang**

**Paper 2011h:** CO<sub>2</sub> Foam Stabilization using Zwitterionic and Nonionic Surfactants — **Muhammad Shahzad Kamal**

**Paper 6fe:** Evaluation of Wax Precipitation Behavior of Wax Deposit: The Effect of Oil Flow Condition — **Xuedong Gao, Qiyu Huang, Yijie Ren, Weidong Li, Xue Dong**

## (202) 3D Printing of Composites Monday, Oct 29, 3:30 PM

David L. Lawrence Convention Center, 333

Holly A. Stretz, Chair  
Jason E. Bara, Co-Chair

**Sponsored by:** 3D Printing

**3:30 Paper 202a:** Cellulose Nanocrystal Thermoplastic Urethane Composite Filament for Fused Filament Fabrication — **Jacob Fallon, Earl J. Foster, Michael J. Bortner**

**3:50 Paper 202b:** Direct Printing of Epoxy-Graphite Composite Ink for Thermal Management Devices — **Roneisha Blakeney, Subramanian Ramakrishnan, Phong Tran, Tarik Dickens**

**4:10 Paper 202c:** Radio Frequency Heating of Carbon Nanotube Composite Materials for Additive Manufacturing — **Charles Sweeney, Mohammad Saed, Micah J. Green**

**4:30 Break**

**4:50 Paper 202e:** Rheology of Cement-Based Pastes for 3-D Printing Applications — **Babajide Y. Onanuga, Matthew S. Whitaker, Joseph J. Biernacki**

**5:10 Paper 202f:** Modeling of Cement Paste for 3-D Printing Applications — **Abdul Salam Mohammad, Joseph J. Biernacki**

## (203) Advanced Problem Solving in the Chemical Industry II

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 407

Zdravko Stefanov, Chair

**Sponsored by:** Young Professionals Committee (YPC)

## (204) Advances in Algal Biorefineries II

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 315

Sridhar Viamajala, Chair  
Robert Gardner, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**3:30 Break**

**3:55 Paper 204b:** Techno-Economic Uncertainty Quantification of Algal-Derived Biocrude Via Hydrothermal Liquefaction Process — **Yuan Jiang, Susanne Jones, Yunhua Zhu, Lesley J. Snowden-Swan, Andrew J. Schmidt, Justin M. Billing**

**4:20 Paper 204c:** Using Produced Water to Grow Microalgae — **Indreesh Badrinarayanan, Jibran Sharieff, Tyler Johannes, Daniel W. Crunkleton**

**4:45 Paper 204d:** Effects of Impurities in Two-Step Vs. One-Step Hydroprocessing of Algae Oils — **Jacob S. Kruger, Earl Christensen, Tao Dong, Gina Fioroni, Philip Pienkos, Robert McCormick**

## (205) Agglomeration and Granulation Processes

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 413

James N. Michaels, Chair  
Stephen L. Conway, Co-Chair

**Sponsored by:** Particle Production and Characterization

**3:30 Paper 205a:** Compartmental Modeling and Simulation Study of Wet Twin Screw Granulator — **Gurmeet Kaur, Themis Matsoukas, Mehakpreet Singh, Jitendra Kumar**

**3:51 Paper 205b:** Developing a Formulation Dependent Mechanistic Kernel to Predict the Granule Size Distribution in a Two Component High Shear Wet Granulation Process — **Indu Muthancheri, Rohit Ramachandran**

**4:12 Paper 205c:** A Model-Based Design of Experiment (MB-DOE) Approach Towards Scale-up of High Shear Wet Granulation Operation — **Maitraye Sen, Salvador Garcia-Muñoz**

**4:33 Paper 205d:** A Population Balance Based Rheological Model for Fresh Cement Paste — **Juan Pablo Gallo-Molina, Ingmar Nopens, Karel Lesage**

**4:54 Paper 205e:** Agglomeration-Driven Product Selection in a Continuously Operated Fluidized-Bed Crystallizer — **Andreas Voigt, Viktoria Wiedmeyer, Kai Sundmacher**

**5:15 Paper 205f:** Roller Compaction Modelling: Pharmaceutical Application — **Ricardo Sousa, Slavomira Doktorovova, Vanessa Sainz, Pedro Valente, Jean-Rene Authelin, Lionel Bardet**

**5:36 Paper 205g:** Anisotropic Mechanical Properties of Compacted Powders with Cohesive Contacts — **Peter Loidolt, Johannes G. Khinast**

## (206) Alternative Fuels Monday, Oct 29, 3:30 PM

David L. Lawrence Convention Center, 405

M. Toufiq Reza, Chair  
Richard H. West, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 206a:** Experimental Study and Modelling of Kinetic Transitions upon Processing of Dimethyl Ether and Methanol to Gasoline (DMTG) at Fluctuating Workloads — **Johannes Kunz, Bettina Kraushaar-Czarnetzki**

**3:52 Paper 206b:** Conversion of Ethanol to Distillate Fuels through Guerbet Condensation — **Nathaniel Eagan, Ashley Wittrig, J. Scott Buchanan, James A. Dumesic, George W. Huber**

**4:14 Paper 206c:** Advanced Reactor Design for CO<sub>2</sub>-Methanation — **Gunnar Ganzer**

**4:36 Paper 206d:** Integration of Renewable Energy Sources into Petroleum Refining for Sustainable Production of Transportation Fuels — **Mohamed Al Jamri, Robin Smith, Jie Li**

**4:58 Paper 206e:** Highly Active and Selective Bifunctional Catalyst for One-Step DME Synthesis By CO<sub>2</sub> Hydrogenation — **Shoujie Ren, Weston R. Shoemaker, Xiaofeng Wang, Zeyu Shang, Naomi Klinghoffer, Shiguang Li, Miao Yu, Xinhua Liang**

**5:20 Paper 206f:** Cobalt Nanoparticles Supported on Graphene for Fischer-Tropsch Synthesis — **Tamara R Mignoli, Thiago L. R. Hewer, Martin Schmal, Rita M. B. Alves**

**5:42 Paper 206g:** Selective Hydrogenation of 5-Hydroxymethylfurfural to 2,5-Dihydroxymethylfuran Using Octahedral Molecular Sieve Support As Catalyst — **Jennifer Dicks, Kathryn Ralphs, Manish Tiwari, Laura Marti, Vivek Ranade, Haresh Manyar**

## (207) Area 2B Plenary: In Honor of Doraiswami Ramkrishna's 80th Birthday (Invited Talks)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 302

Seth Huggins, Chair  
Thomas Vetter, Co-Chair  
Meenesh R. Singh, Co-Chair

**Sponsored by:** Crystallization and Evaporation

**3:30** Introductory Remarks - in Honor of Doraiswami Ramkrishna's 80th Birthday

**3:40 Paper 207a:** Insulin Exits Skeletal Muscle Capillaries By Fluid-Phase Transport — **Jamey D. Young**

**4:05 Paper 207b:** Pharmacometric Model Guided Control for Improved Therapeutic Exposure — **Eric Sherer**

**4:30 Paper 207c:** Spatiotemporal Dynamics of the Human Gut Microbiome — **Prasad S. Dhurjati**

**4:55 Paper 207d:** Sequence Specific Modeling of *E. coli* Cell-Free Protein Synthesis — **Jeffrey Varner**

**5:20 Paper 207e:** Viewing Crystallization from the World of Population Balances — **Doraiswami Ramkrishna**

**5:45** Concluding Remarks - in Honor of Doraiswami Ramkrishna's 80th Birthday

## (208) Brewing Education and Training

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 329

Catherine E. Brewer, Chair  
David Rockstraw, Co-Chair

**Sponsored by:** Miscellaneous

**3:30 Paper 208a:** The Role of Industry in Helping Shape University Brewing Education Programs — **Andrew McMichael**

**3:50 Paper 208b:** On the Origin and Evolution of Brewing Science and Technology at Villanova — **Michael A. Smith**



**4:10 Paper 208c:** Designing a Brewery Engineering Minor within Chemical Engineering to Meet MBAA Specifications — *Catherine E. Brewer, Stephen Taylor, David Rockstraw*

**4:30 Paper 208d:** From Concept to Class: Pitt's Engr 1933 – Engineering a Craft Brewery — *Robert S. Parker*

**4:50 Paper 208e:** Brewing and Distilling: Alive and Well in Northwest Arkansas and the University — *Abdollah Mosleh, Jesse Roberts, Lauren F. Greenlee, Wesley Stites, Shannon L. Servoss*

**5:10 Paper 208f:** Optimization of Aroma Profiles through Selective Removal of Off-Flavors: An Exemplary Study in Alcohol-Free Beers — *Deborah C. Gernat, Fiona M. Swinkels, Maxime M. Penning, Eric Brouwer, Marcel Ottens*

**5:30 Paper 208g:** Heat Transfer in a Recirculating Infusion Mash System — *Justin Federici, Clay Sutton, Hari Nair, Phillip K. Schoch, Sundar Narayanan, Anastasios Skoulidas*

#### (209) Carbon Dioxide Capture Technologies and Their Use II

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 319

Sunil Hangal, Chair  
Gonzalo Guillén-Gosálbez, Co-Chair

**Sponsored by:** Climate Change

**3:30 Paper 209a:** Life Cycle Analysis of Carbon Capture Retrofit Using the Petra Nova Model — *Derrick Carlson, Gregory Cooney*

**3:49 Paper 209b:** A Model for Packed and Fluidized Bed Absorbers with Micro-Encapsulated CO<sub>2</sub> Sorbents — *Katherine Hornbostel*

**4:08 Paper 209c:** Flue Gas to Food Security: Radical Reductions in Greenhouse Water Usage through Direct Utilization of CO<sub>2</sub> — *Neil Thomas Stacey, James A. Fox, Diane Hildebrandt*

**4:27 Paper 209d:** Redesigning the Regulated Power Plant: Optimizing Energy Allocation to Electricity Generation, Carbon Capture, and Water Treatment Processes at Coal-Fired Power Plants — *Daniel Gingerich, Meagan Mauter*

**4:46 Paper 209e:** Cost Analysis Model for Air Capture Sorbents — *Habib Azarabadi, Klaus Lackner*

**5:05 Paper 209f:** A New 12-Step Climate Change Mechanism, based on Formation of Carbon Dioxide Hydrates Around Deep Ocean Submarine Volcanoes and Hydrothermal Vents — *Gerard Caneba*

**5:24 Paper 209g:** Experimental Framework for Understanding Intermolecular Interactions in Carbon Dioxide-Water Mixtures for EOR and Storage — *Richa Sharma, Quincy K. Elias, T. S. Ramakrishnan*

#### (210) Chemical and Catalytic Conversions and Processes for Renewable Feedstocks

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 316

Michael Mullins, Chair

**Sponsored by:** Sustainable Biorefineries

**3:30 Paper 210a:** Catalytic Upgrading of Pyrolysis Vapor at Bench Scale with Platinum on Titania — *Richard J. French, Kristiina Iisa, Kellene A. Orton, Calvin Mukarakate, Joshua A. Schaidle*

**3:55 Paper 210b:** Catalytic Pyrolysis of Chitin over H-ZSM-5 — *Harsha Gogulapati, Hsi-Wu Wong*

**4:20 Paper 210c:** Assessment of Hydrothermal Liquefaction Oil with Catalytic Upgrading for Renewable Fuel and Chemical Production — *LiLu Funkenbusch, Michael Mullins, Lennart Vamling, Tallal Belkheiri, Nattapol Srettiwat, Olumide Winjobi, David R. Shonnard, Tony N. Rogers*

**4:45 Paper 210d:** Fatty Acid Methyl Ester Production Via Ferric Sulfate Catalyzed Interesterification — *Lindsay Soh, Yuan Tian, Junwei Xiang, Christopher Verni*

**5:10 Paper 210e:** Impact of Organic and Inorganic Impurities on Catalyst Performance and Finished Product in the Production of Acrylonitrile from Biomass — *Swanand Tupsakhare, Zora Govedarica, Jadid E. Samad, Amit Goyal*

#### (211) Chemical Engineers and Policy-Making

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 331

Quinta Warren, Chair

**Sponsored by:** Management Division

**3:30 Paper 211a:** Career Opportunities for Engineers in Science and Technology Policy — *Alexis McKittrick, Leslie Abrahams*

**3:55 Paper 211b:** Chemical Engineering and Environmental Policy — *Mary Ellen Ternes*

**4:20 Paper 211c:** A Pathway to a Career in the Federal Government — *Kelly Fleming*

**4:45 Paper 211d:** Data Is the New Black: Information Is Critical to Policy-Making — *Elizabeth Sendich*

**5:10 Paper 211e:** From Lab Coats to Waistcoats — *Samuel M Goodman*

#### (212) Community-Based Water Treatment Innovations

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 320

Robert W. Peters, Chair  
Kashinath Banerjee, Co-Chair  
Matthew L. Alexander, Co-Chair

**Sponsored by:** Water

**3:30 Paper 212a:** Marine Exoskeleton-Based Biosorption of Heavy Metals: Performance and Cost Analysis — *Carolina Londono Zuluaga, Lucian A. Lucia, Hasan Jameel, Ronalds Gonzalez*

**3:55 Paper 212b:** RO Denitrification and Desalting of Impaired Brackish Water in Remote Communities — *Jin Yong Choi, Abdullah Aleidan, Yian Chen, Anditya Rahardianto, Madelyn Glickfeld, Yoram Cohen*

**4:20 Paper 212c:** Optoelectrokinetic Trapping of *Escherichia coli* in Water — *Uzumma O. Ozeh, A. G. Agwu Nnanna, Justus C. Ndukaife*

**4:45 Paper 212d:** Biocomposite Material from Figue and Iron Nanoparticles As Adsorbent for Mercury Removal from Aqueous Solutions: Kinetic and Equilibrium Studies — *Karen Giovanna Bastidas Gómez, Cesar Augusto Sierra Avila, Hugo Ricardo Zea Ramirez*

#### (213) Computational Modeling and Validation for Fluidization Processes

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 415

Reza Mostofi, Chair  
Mikio Sakai, Co-Chair

**Sponsored by:** Fluidization and Fluid-Particle Systems

**3:30 Paper 213a:** Development of CFD-DEM Coupling Model for Particles-Liquid-Gas Flow — *Kimiaki Washino, Tetsushi Kaji, Yoshiaki Matsuno, Ei L. Chan, Takuya Tsuji, Toshitsugu Tanaka*

**3:48 Paper 213b:** Meso-Scale Nonequilibrium Characteristics in a Bubbling Fluidized Bed — *Haifeng Wang, Yanpei Chen, Wei Wang*

**4:06 Paper 213c:** Development of Drift Velocity Transport Equation for Filtered Drag Force Model — *Yundi Jiang, Ali Ozel, Jari Kolehmainen, Yannis G. Kevrekidis, Sankaran Sundaresan*

**4:24 Paper 213d:** Numerical Study on a Gas-Solid Flow in an Arbitrary Shape Boundary Including Thin Plates — *Kazuya Takabatake, Mikio Sakai*

**4:42 Paper 213e:** Application of a Modified CFD-PBM Method to the Simulation of a Slurry Bed Reactor — *Wu Su, Yingya Wu, Xiaogang Shi, Xingying Lan, Jinsen Gao*

**5:00 Paper 213f:** Catalytic Propane Oxidative De-Hydrogenation with High Propylene Selectivity in a Downer Fluidized Bed Reactor: Kinetics and CPFD Simulation — *Samira Rostom, Imtiaz Ahmed, Hugo de Lasa*

**5:18 Paper 213g:** An Orthogonal Recursive Bisection (ORB) Based Time Advancement Algorithm for CFD-DEM Solvers — *Hariswaran Sitaraman, Ray Grout*

**5:36 Paper 213h:** Effect of Collision Angle on Particle-Particle Adhesion of Colliding Particles through Liquid Droplet — *Hideya Nakamura, Hiroyuki Kan, Satoru Watano*

#### (214) Developments in Extractive Separations: Processes

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 303

Glenn Shivelor, Chair  
Guangsheng Luo, Co-Chair  
George S. Goff, Co-Chair

**Sponsored by:** Extractions

**3:30 Paper 214a:** Silver Recovery from Catalysts Using a Leaching and Emulsion-Liquid-Membrane Hybrid Process — *Saeed Laki, Ahmad Arabi Shamsabadi, Farzad Seidi, Masoud Soroush*

**3:55 Paper 214b:** Upgrading of Bio-Oil As Transportation Fuel Using Water/Oil Based Extraction — *Rozzeta Dolah, Rohit Karnik, Halimatun Hamdan*

**4:20 Paper 214c:** Astaxanthin and Triglyceride Co-Products from Microalgae with Sequential Supercritical Carbon Dioxide Selective Extraction Schemes — *Thomas Kwan*

**4:45 Paper 214d:** Integration of Enzymatic Reactions into Continuous Countercurrent Extraction Processes with Mixed Surfactant Solutions — *Irina Smirnova, Oliver Fellechner*

**5:10 Paper 214e:** Enhanced Wet Extraction of DHA Using Room-Temperature Ionic Liquids — *Yujie Zhang*

**5:35 Paper 214f:** Deep Desulfurization of Fuels Using Imidazolium Anion-Based Ionic Liquids — *Lu Wei, Weidong Liu, Mingxia Li, Fan Zhang, Zhiyong Zhou, Zhongqi Ren*

**(215) Developments in Unconventionals: Shale Gas, LNG, CNG, and LPG**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 323

Sheima J. Khatib, Chair  
Belma Demirel, Co-Chair

**Sponsored by:** Alternate Fuels and New Technology

**3:30 Paper 215a:** Investigation of Effects of Subcritical Water As Fracturing Fluid on Hydraulic Fracturing and Fracture Permeability of Shale — *Md. Rifat Hasan, M. Toufiq Reza*

**3:48 Paper 215b:** Drag Model Development and 3-Phase Simulation of Methane Production from a Gas Hydrate Reservoir — *Deniz Hinz, Hamid Arastoopour, Javad Abbasian*

**4:06 Paper 215c:** Badak LNG Process Transformation: Challenges in Handling Leaner Feed Gas — *Robby S. Dharmawan, Ferry A. Perdana*

**4:24 Paper 215d:** Natural Gas Liquids (NGL)- Fractionate or NOT to Fractionate at the Gas Processing Plant — *Bijal Gangar, Ali A. Pilehvari*

**4:42 Paper 215e:** Optimal Operation for LNG Ship Tank Commissioning and Loading Via Rigorous Dynamic Simulations — *Yogesh Kurle, Qiang Xu, Srinivas Palanki*

**5:00 Paper 215f:** Greenhouse Gas Footprints of Transportation Fuels Manufactured from Natural Gas Liquids Derived from Shale Gas — *Qining Chen, Jennifer B. Dunn, David T. Allen*

**5:18 Paper 215g:** Effect of Temperature in Methane Dehydroaromatization over Mo Supported on Sulfated Zirconia Catalysts — *Swarom Kanitkar, Ashraf Abedin, Srikar Bhattar, James J. Spivey*

**5:36 Paper 215h:** Probing the Influence of Structural Changes on the Microstructural Evolution in Shale on Heating using Multi-Scale X-ray Scattering Measurements — *Greeshma Gadikota, Meishen Liu*

**(216) Efficient Processing of Lignin to Bioproducts and Biofuels II**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 318

Bin Yang, Chair  
Arthur J. Ragauskas, Co-Chair  
Joshua Yuan, Co-Chair  
Ning Sun, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**3:30 Paper 216a:** Characterizing Lignin from a Low Temperature Hydrotropic Process for Valorization — *J.Y. Zhu*

**3:45 Paper 216b:** Statistical Modeling to Optimize Lignin Conversion to Polyhydroxybutyrate By *Cupriavidus Necator* — *Mengxing Li, Mark R. Wilkins, Kent Eskridge*

**4:00 Paper 216c:** Effect of Pretreatment Conditions on the Structure of Celf Lignin — *Yun-Yan Wang, Priya Sengupta, Charles E. Wyman, Charles M. Cai, Arthur J. Ragauskas*

**4:15 Paper 216d:** Innovative Design to Transform Waste Valorization through Co-Processing of Lignin and Residual Saccharides (CLARS) in an Integrated Biorefinery — *Zhi-Hua Liu, Arthur J. Ragauskas, Joshua Yuan*

**4:30 Paper 216e:** The Application of Stochastic Optimization in Lignin Depolymerization Process — *Hanxi Bao, Zhiqiang Zhu, Guanghui Lan, Zhaohui Tong*

**4:45 Paper 216f:** Towards Biocatalytic Lignin Valorization in Aqueous Ionic Liquids Using Thermophilic Laccases — *Joseph Stevens, Justin Mobley, Lalitendu Das, David Rodgers, Jian Shi*

**5:00 Paper 216g:** Reductive Mechanocatalytic Depolymerization of Lignin — *Andrew Tricker, Carsten Sievers*

**5:15 Paper 216h:** Depolymerization of Lignin to Mono-Aromatic Compounds over Solid Acid Catalysts with Hydrogen — *Hao Ruan, Bin Yang*

**(217) Electrocatalysis and Photoelectrocatalysis III: Hydrogen Evolution Reaction**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 401

Karthish Manthiram, Chair  
Ben Meekins, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 217a:** Integrating Non-Precious Metal H<sub>2</sub> Evolution Catalysts into Water Electrolyzers and Photoelectrochemical Water-Splitting Devices — *Thomas F. Jaramillo*

**3:48 Paper 217b:** When Electrocatalysis Matters and When It Does Not: Unexpected Observations in Water Electrolysis and Flow Battery Energy Storage — *James R. McKone*

**4:06 Paper 217c:** Understanding the Role of Adsorbed Hydroxide in Reversible Hydrogen Reactions — *Saad Intikhab, Joshua Snyder, Maureen H. Tang*

**4:24 Paper 217d:** Electrocatalysis at Buried Interfaces — *Daniel Esposito*

**4:42 Paper 217e:** Density-Functional-Theory Studies of Face-Centered-Cubic Tungsten Carbide and Pt Core-Shell Nanoparticles Catalysts for the Hydrogen Evolution Reaction — *Akash Jain, Ashwin Ramasubramaniam*

**5:00 Paper 217f:** Kinetic Investigation of Nickel-Iron Layered Double Hydroxide for Hydrogen Evolution in an Alkaline Electrolyte — *Aisha Alobaid, Chunsheng Wang, Raymond A. Adomaitis*

**5:18 Paper 217g:** BiVO<sub>4</sub>/WO<sub>3</sub> Photoanodes for Chloride Oxidation with Simultaneous H<sub>2</sub> Production — *Alan Rassoolkhani, Wei Cheng, Austin McKee, Jonathan Koonce, Abdulsattar Alsaedi, Syed Mubeen*

**5:36 Paper 217h:** On the Combustion Synthesis and Characterization of Ga<sub>2</sub>Zn<sub>1-γ</sub>OyN<sub>1-γ</sub> for Water Splitting Applications — *Austin Kennedy, Ben Meekins*

**(218) Emerging Trends in Smart Manufacturing (sponsored by CEMII)**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 408

Haresh Malkani, Chair

**Sponsored by:** Next-Gen Manufacturing

**3:30 Paper 218a:** About CEMII —

**4:00 Paper 218b:** Overview of R&D projects advancing CEMII's Mission —

**4:30 Panel discussion –** Democratization of Smart Manufacturing

**(219) Experimental Methods and Characterization of Adsorbent Materials**

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 311

Marcus Mello, Chair  
Gennady Gor, Co-Chair  
Sasidhar Gumma, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**3:30 Paper 219a:** Isothermic Heats of Adsorption of Water on Zeolites — *Vladimir Martis, Juliane Willkomm, Alexandra Lieb*

**3:50 Paper 219b:** Hierarchical Bayesian Estimation for Adsorption Isotherm Parameter Determination and Applications to CO<sub>2</sub> capture — *Chunkai Shih, Jongwoo Park, David S. Sholl, Matthew Reaff, Tomoyuki Yajima, Yoshiaki Kawajiri*

**4:10 Paper 219c:** The Influence of Compositions and Defects on Vibrational and Optical Properties of Sodalite through Density Functional Theory — *Amir M. Mofrad, Caio Peixoto, Heather K. Hunt, Karl D. Hammond*

**4:30 Paper 219d:** Pore Structure Characterization of MOF-Based Materials By Gas Adsorption — *F. Silvio P. Dantas, Katie A. Cychoz, Matthias Thommes, Alexander Neimark*

**4:50 Paper 219e:** Assessment of Options for Determining the Total Adsorption Uptake from Liquid Solution: Alkane- $\alpha,\omega$ -Diols/(Water or Ethanol) Onto Silicalite-1 — *Robert F. DeJaco, Matheus Dorneles de Mello, Bahman Elyassi, Nitish Mittal, Michael Tsapatsis, J. Ilja Siepmann*

**5:10 Paper 219f:** Measurement of Water Adsorption Kinetics Using the Zero Length Column — *Alessio Centineo, Stefano Brandani*

**5:30 Paper 219g:** Impact of the Addition of Polyethylene Glycol (PEG) on Amine Efficiency and Heat of Sorption in Polyethylenimine (PEI)/Silica Sorbents — *Linxi Wang, Mohammad Al-Aufi, Liyuan Xie, Robert Rioux*

## (220) Faculty Candidates in CoMSEF

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 308

Amir Haji-Akbari, Chair  
Jeremy C. Palmer, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**3:30 Paper 220a:** Computationally-Efficient High-Throughput Screening of Nanoporous Materials for Hydrogen Storage — **N. Scott Bobbitt**, Benjamin Bucior, Arun Gopalan, Neda Bagheri, Randall Q. Snurr

**3:45 Paper 220b:** Computational Design of Efficient Catalysts for CO<sub>2</sub> Hydrogenation — **Jingyun Ye**

**4:00 Paper 220c:** Quantum Mechanics Based Multiscale Reactive Simulations of Materials and Processes — **Saber Naserifar**

**4:15 Paper 220d:** Reaction Ensemble Monte Carlo Simulations of Protic Ionic Liquid Formation — **Ryan Gotchy Mullen**, Edward Maginn

**4:30 Paper 220e:** Estimation of Nucleation Barriers for Colloidal Crystals from Computer Simulations — **Antonia Statt**, Peter Virnau, Kurt Binder

**4:45 Paper 220f:** Replicating the Static and Dynamic Behavior of a Hybrid Fluid Via Relative Resolution — **Aviel Chaimovich**, Christine Peter, Kurt Kremer

**5:00 Break**

**5:15 Paper 220h:** Using Advanced Field-Based Approaches to Predict Polymer Nanocomposite Phase Behavior — **Jason P. Koski**, Amalie L. Frischknecht, Robert A. Riggelman

**5:30 Paper 220i:** A Graph-Based Approach for Systematic Molecular Coarse-Graining — **Michael Webb**, Juan de Pablo

**5:45 Paper 220j:** Data-Driven Modeling in Molecular Science and Chemical Engineering — **Joseph S. Gomes**

## (221) Free Forum on Engineering Education: Junior and Senior Years II

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 411

Daniel Knight, Chair  
Sandra L. Pettit, Co-Chair

**Sponsored by:** Undergraduate Education

**3:30 Paper 221a:** A Curriculum-Wide Strategy for Student Teaming Skills Development in Engineering — **Natasha Mallette**, Christine Kelly, Michelle Bothwell, Milo D. Koretsky

**3:47 Paper 221b:** Applying Engineering Optimization Principles to Engineering Education: Optimization of a Student Project Experience's Design and Implementation — **Kristen M. Wilding**, Ford Hayley, Bradley C. Bundy

**4:04 Paper 221c:** An Interdisciplinary Research Program for Undergraduate within the Functional Materials and Manufacturing Institute at University of South Florida — **John N. Kuhn**, Venkat R. Bhethanabotla

**4:21 Paper 221d:** Vanderbilt's Process Innovation Center: A Multipurpose Facility for Teaching Chemical Engineering Lab and Design Courses — **Russell F. Dunn**, G. Kane Jennings, Scott A. Guelcher

**4:38 Paper 221e:** Integrating Laboratory Experiments into Chemical Engineering Core Courses — **David M. Griffin**, Mark B. Shiflett

**4:55 Paper 221f:** Biochemical Engineering Lab Course: Preparing Undergraduates for the Biotechnology Industry — **Frederick Twigg**, Shannon Ciston, Esayas Kelkile, Wenjun Zhang

**5:12 Paper 221g:** Case Studies As Vehicles for Enhancing Students' Perceptions of the Broad Relevance of Biochemistry in Chemical Engineering — **Ian Schneider**, Laura Jarboe, Thomas J. Mansell, Reuben Peters, Zengyi Shao

**5:29 Paper 221h:** Student-Driven Process Oriented Guided Inquiry Learning (POGIL) Based Biochemical Engineering Technical Elective Course — **Anju Gupta**

## (222) Graduate Student Competition in Microbiointerface Research

**Monday, Oct 29, 3:30 PM**

Westin Convention Center, Pennsylvania East

Anita Shukla, Chair  
Huan Gu, Co-Chair  
Cesar de la Fuente-Nunez, Co-Chair

**Sponsored by:** Microbes at Biomedical Interfaces

**3:30 Introductory Remarks**

**3:35 Paper 222a:** Sensitizing Bacterial Cells to Antibiotics through Dynamic Topography-Triggered Biofilm Detachment — **Sang Won Lee**, Huan Gu, James Kilberg, Dacheng Ren

**3:55 Paper 222b:** The Role of Flagellar Motor Reversals in Swarming in *Escherichia coli* — **Katie Ford**, Jyot Antani, Pushkar Lele, Aravindh Nagarajan

**4:15 Paper 222c:** Pseudomonas Aeruginosa Single-Cell Level Heterogeneity, Investigated Via Drop-Based Microfluidics — **Shawna Pratt**, Tatsuya Akiyama, Geoffrey Zath, Kerry Williamson, Michael Franklin, Connie B. Chang

**4:35 Paper 222d:** Differential Response of Mucoic and Non-Mucoic *Pseudomonas Aeruginosa* Isolates to Interfacial Confinements — **Sricharani Balmuri**, Nicholas Waters, Tagbo H.R. Niepa

**4:55 Paper 222e:** Bloodmeal-Induced Inhibition of *Plasmodium* Infection in Mosquito Vectors Using the Microbial Symbiont *Asaia* — **Jackie Shane**, David Lampe

**5:15 Paper 222f:** Dynamics of Biofilm Elimination on Thermally Shocked Biomedical Surfaces — **Haydar Aljaafari**, Erica Ricker, Eric Nuxoll

**5:35 Paper 222g:** Modelling Microbial Microenvironments through Encapsulation of Synthetic Communities — **Shanna Davidson**, Erin. K Hunter, Tagbo H.R. Niepa

**5:55 Concluding Remarks**

## (223) Green Chemistry and Engineering

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 309

Lindsay Soh, Chair  
Christina Tang, Co-Chair

**Sponsored by:** General

**3:30 Paper 223a:** Circular Economy Methods of Preparing Fragrance Compounds — **Sunitha Tadepalli**, Geatesh Tampy, Zhe Guo

**3:52 Paper 223b:** Optimizing Process Parameters for Stable Inorganic Nanoparticle Production in a Multi-Vessel Reactor System Using Microalgae — **Ashiqur Rahman**, Tushar Nemade, Shishir V Kumar, Adarsh Bafana, Si Amar Dahoumane, Clayton S Jeffryes

**4:14 Paper 223c:** Catalytic Gasification for Waste Management: Selectivity of Oxidation Reactions for Model Polymers — **Mason Lang**, Kristen Reyes, Michael Matrona, Eric Lange, Brianna DeMattia, Uchechukwu Obiako, Jorge E. Gatica

**4:36 Paper 223d:** Sustainable Synthesis of Glassy Liquid Crystals As Advanced Optical Materials — **Jason U. Wallace**, Alexander Shestopalov, Shaw H. Chen

**4:58 Paper 223e:** Informatics for Green and Sustainable Nanomaterials — **Nastassja Lewinski**

## (224) Heat Transfer in Particulate Systems

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 414

Emad Abbasi, Chair  
Maulik Mehta, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**3:30 Paper 224a:** Spatially-Averaged Models for Heat Transfer in Gas-Solid Flows — **Stefanie Rauchenzauner**, Simon Schneiderbauer

**4:00 Paper 224c:** Effect of Baffles on the Rate of Heat Transfer in Rotating Drums — **Bereket Yohannes**, Calvin Kim, William G. Borghard, Fernando. J Muzzio, Benjamin Glasser, Alberto M. Cuitino

**4:30 Paper 224e:** A Novel Approach for Radiative Thermal Exchange in Coupled Particle Simulations — **Thomas Forger**, Johannes G. Khinast, Stefan Radl

**5:00 Paper 224f:** Experimental Studies of Thermal Properties of Packed Powder Beds — **Anna Nachtigal**, Calvin Kim, Bereket Yohannes, Fernando. J Muzzio, William G. Borghard, Benjamin Glasser, Alberto M. Cuitino

**5:30 Paper 224g:** Particle Dynamic Simulations of Heat Transfer in a Bladed Mixer: Effect of Material and Process Parameters — **Clara Hartmanshenn**, Benjamin J. Glasser

## (225) How Summer School Improved My Teaching

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 409

Daniel D. Burkey, Chair  
Jennifer Weiser, Co-Chair

**Sponsored by:** Professional Development Committee Liaison

**3:30 Paper 225a:** Getting Active: How the ASEE Summer School Shaped My Teaching Practices — **Jennifer Weiser**

**3:48 Paper 225b:** Incorporating Teaching Methods from the ASEE Summer School during My First Year on the Job — **Adrianne M. Rosales**



**4:06 Paper 225c:** Combining the Luck of the Draw with Individual Accountability in Team-Based Learning — *Erick S. Vasquez*

**4:24 Paper 225d:** Improvements in Teaching Core Undergraduate Courses after Chemical Engineering Summer School 2017 — *Michael M. Nigra*

**4:42 Paper 225e:** How Summer School Improved Our Safety Education in the Unit Operations Laboratory — *Tracy Carter, M. Jane Brennan, Elizabeth Hill, Samira M. Azarin, Amy Karlsson*

**5:00 Paper 225f:** Opportunities and Obstacles: Using Board Games to Engage Students in Deeper Analysis of Societal Issues with (Potential) Genetic Engineering Solutions — *Elif E. Miskioglu*

**5:18 Paper 225g:** Flipping the Classroom to Increase Student Engagement in an Elective Biochemical Engineering Course — *Adam Melvin*

**5:36 Paper 225h:** The Startup Method to Managing Large Classes – a Technique Inspired By Asee Summer School 2017 — *Nigel Reuel*

#### (226) In Honor of Neal Chung I: Gas Separation

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 304

Ivy Huang, Co-Chair  
Haiqing Lin, Co-Chair  
Glenn Lipscomb, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 226a:** Gas Separation Properties of Novel Poly(benzimidazole)s — *Benny D. Freeman, Joshua D. Moon*

**3:52 Paper 226b:** Graphene Oxide Membranes for Gas Separation – Gas Transport Mechanism — *Jerry Y.S. Lin*

**4:14 Paper 226c:** Ionic Liquid-Based Gel Membranes with Tough Double-Network for CO<sub>2</sub> Separation — *Hidetoshi Matsuyama*

**4:36 Paper 226e:** Designing Sorption-Enhanced Mixed Matrix Membranes for H<sub>2</sub>/CO<sub>2</sub> Separation Using an Integrated Experimental and Modeling Approach — *Haiqing Lin*

**4:58 Paper 226f:** Optimizing Carbon Capture with Membrane Processes — *Norfanila Che Mat, Glenn Lipscomb*

**5:20 Paper 226g:** Haifeng Power Plant CO<sub>2</sub> Capture Demo Unit — *Ivy Huang*

**5:42 Paper 35d:** PVDF Hollow Fibers with Novel Sandwich Structure and Superior Wetting Resistance for Vacuum Membrane Distillation — *Jian Zuo, Neal Tai-Shung Chung*

#### (227) In Honor of Peter Monson II (Invited Talks)

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 307

David A. Kofke, Chair  
David M. Ford, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**3:30 Paper 227a:** A Celebration of My 15+ Year Collaboration with Peter Monson on Simulating the Self Assembly of Nanoporous Materials: Are We Sipping from the Holy Grail? — *Scott M. Auerbach*

**3:48 Paper 227b:** Confinement-Induced Compression and High Pressure Phases in Nanopores — *Keith E. Gubbins, Cody K. Addington, James Mansell, Malgorzata Sliwinska-Bartkowiak, Deepthi Srivastava*

**4:06 Paper 227c:** My Research Adventures with Pete Monson — *Peter T. Cummings*

**4:24 Paper 227d:** Monte Carlo Simulation of Percolation Properties, Including Cluster Numbers and Elastic Backbones — *Robert M. Ziff*

**4:42 Paper 227e:** Cyclic and Polymeric Rotaxanes — *Edith Sevick*

**5:00 Paper 227f:** The Treatment of Pair Correlations in an Augmented Mean-Field Density Functional Theory of a Simple Model Liquid Crystal — *Martin Schoen, Andrew J. Haslam, George Jackson*

**5:18 Paper 227g:** Molecular Modeling of Nanoparticle Permeation in Lipid Membranes for Drug Delivery Applications — *Priyanka Oroskar Sharma, Cynthia J. Jameson, Sohail Murad*

**5:36 Paper 227h:** Phase Diagrams By Computer Simulations: A Good School for Force Fields — *Carlos Vega*

**(228) In Honor of the 2017 Wilhelm Award Winner II (Invited Talks)**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 406

Matthew Neurock, Chair  
Robert J. Davis, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 228a:** The Drive for Advantaged on-Purpose Propylene — *Billy B. Bardin, Matt Pretz, Lin Luo*

**3:55 Paper 228b:** Solvent Effects in Acid-Catalyzed Reactions of Biomass-Derived Oxygenates — *James Dumesic, Max A. Mellmer, Chotitath Sanpitakseree, Benginur Demir, Peng Bai, Kaiwen Ma, Theodore Walker, Alex Chew, Huixiang Li, Z. Conrad Zhang, George W. Huber, Reid Van Lehn, Matthew Neurock*

**4:20 Paper 228c:** Synthesis of Chiral Molecular Sieves: A 30 Year Journey — *Mark E. Davis*

**4:45 Paper 228d:** Atom Trapping: A Novel Approach to Generate Thermally Stable and Regenerable Single Atom Catalysts — *Abhaya K. Datye, Andrew T. DeLaRiva, Xavier Isidro Pereira Hernandez, Haifeng Xiong, Deepak Kunwar, Christopher Ryan Riley, Eric J. Peterson, Yong Wang*

**5:10 Paper 228e:** Spectroscopic and Transient Kinetic Analyses of Metal Catalysts for the Conversion of Oxygenates — *Robert J. Davis*

#### (229) International House of Chemical Engineers

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 410

Said AbuBakr, Chair  
Luke Achenie, Co-Chair  
Yinlun Huang, Co-Chair  
Marcel A. Liauw, Co-Chair

**Sponsored by:** Education

**3:30 Paper 229a:** Experiences of Embedding Safety throughout a Chemical Engineering Program — *Eva Sorensen, Michaela Pollock*

**3:48 Paper 229b:** Preparing Students for Design Experiences in a Global Setting — *Randy S. Lewis, Terri Bateman, Carol Ward*

**4:06 Paper 229c:** Research Symposium for Engaging Students in Undergraduate Research — *Tomás-Eduardo Chávez-Miyauchi, Sara Betsabé Morales Luna, Luis Romeo Guillén Palacio*

**4:24 Paper 229d:** The Formation of the Dakar American University of Science and Technology in Senegal — *Quinta Nwanosike Warren*

**4:42 Paper 229e:** Smart Materials and Microfluidics Research Practicum for Chemical Engineering Students: A Case Study — *Artem Bezrukov*

**5:00 Paper 229f:** Teaching Pharmaceutical cGMP Concepts Using 3D Manufacturing Plant — *Shin Yee Wong*

**5:18 Paper 229g:** Global Human Engineering Projects and Initiatives to Enhance Student Learning and Strengthen the Curriculum and Program Accreditation Efforts — *Laura Ford, Zenaída Otero Gephardt, Christi Patton Luks*

**5:36 Paper 229h:** An Example of How the Scientific Research Provide New Material in the Teaching of Transport Phenomena — *Benito Serrano Rosales, Hugo de Lasa, Brandon Alexis Garcia Saucedo Sr., Dennis Misael Ramirez Estrada Sr., Abraham Carrillo Campos Sr., Alfonso Talavera Sr., Salvador Escobedo Jr.*

#### (230) Mathematical Modeling of Transport Processes

**Monday, Oct 29, 3:30 PM**  
Omni William Penn Hotel, Conference Center B

Norman Loney, Chair  
Sara Hashmi, Co-Chair

**Sponsored by:** Transport Processes

**3:30 Paper 230a:** Spontaneously Oscillating Menisci: Maximizing Evaporative Heat Transfer By Inducing Condensation — *Thao Nguyen, Joel L. Plawsky, Peter C. Wayner Jr.*

**3:45 Paper 230b:** Deep Learning Physical Phenomena — *Joseph S. Gomes, Vijay Pande*

**4:00 Paper 230c:** Solution of the Boltzmann Transport Equation Via Numerical Tensor Methods — *Arnout Boelens, Daniele Venturi, Daniel Tartakovsky*

**4:15 Paper 230d:** Finite Element Analysis of Heat Transfer in a Solid State Reaction System — *Venkata V. K. Doddapaneni, Sidney Lin*

**4:30 Paper 230e:** Ignition of Energetic Material Using a Subscale Frank-Kamenetskii Model with Detailed Chemical Kinetics — *Nikolai D. Petsev, Xia Ma, Bryan Henson, Brad Clements*



**4:39 Paper 235e:** A CO<sub>2</sub> Utilization Approach Towards the Synthesis of Terephthalic Acid — **Samuel Thompson**, Marty Lail, Qinghe Zheng, Thomas Gohndrone

**4:57 Paper 235f:** Catalytic CO<sub>2</sub> Hydrogenation to C<sup>2+</sup> Hydrocarbons — **Wenjia Wang**, Xiaoxing Wang, Xiao Jiang, Chunshan Song

**5:15 Paper 235g:** Effect of CO<sub>2</sub> Source and Concentration on the Catalyst Performance and Economics of Ethane Oxidative Dehydrogenation to Ethylene — **Jadid Samad**, Amit Goyal

**5:33 Paper 235h:** Utilization of CO<sub>2</sub> Towards Solar Fuel Production Via Ferrite Based Redox Reactions — **Rahul Bhosale**, Gorakshnath Takalkar

**(236) PI Topical Conference Plenary: A Look Inside the RAPID Manufacturing Institute, Co-Hosted by RAPID and F&PD**

**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 335

James Bielenberg, Chair

**Sponsored by:** Process Intensification & Modular Chemical Processing

**3:30 Paper 236a:** RAPID Manufacturing Institute Overview — **James Bielenberg**

**3:40 Paper 236b:** RAPID's Education & Workforce Development Efforts — **Ashley Smith-Schoettker**

**3:50 Paper 236c:** RAPID Focus Area: Intensified Process Fundamentals — **Dionisios Vlachos**

**4:10 Paper 236d:** RAPID Focus Area: Modeling & Simulation —

**4:30 Paper 236e:** RAPID Focus Area: Module Manufacturing — **Brian Paul**

**4:50 Paper 236f:** RAPID Focus Area: Renewable Bioproducts — **Robert C. Brown**

**5:10 Paper 236g:** RAPID Focus Area: Natural Gas Upgrading — **Scott Klara**

**5:30 Paper 236h:** RAPID Focus Area: Chemicals and Commodity Processing — **Thomas F. Edgar**

**(237) Poster Session: Fluid Mechanics**

**Monday, Oct 29, 3:30 PM**  
Omni William Penn Hotel, Frick

John M. Frostad, Chair  
Travis W. Walker, Co-Chair

**Sponsored by:** Fluid Mechanics

**Paper 237a:** Dynamics of Spheroidal Capsules in Microfluidic Channels — **Abdollah Koolivand**, Panagiotis Dimitrakopoulos

**Paper 237b:** Precise Control over the Position and Orientation of Anisotropic Colloidal Particles Using a Stokes Trap — **Dinesh Kumar**, Anish Shenoy, Charles Young, Songsong Li, Charles E. Sing, Charles M. Schroeder

**Paper 237c:** Generalized Langevin Dynamics for Adhesion of a Polymer-Grafted Nanoparticle to Cell — **Yu-Wen Wu**, Hsueh-Te Chung, Hsiu-Yu Yu

**Paper 237v:** Effective Viscosity of a Dilute Emulsion of Spherical Drops containing Soluble Surfactant — **Rajarshi Sengupta**, Lynn Walker, Aditya S. Khair

**Paper 237d:** Probing the Rheological, Electrical, and Microstructural Properties of Complex Fluids with Dielectric Rheosans — **John K. Riley**, Jeffrey J. Richards, Norman J. Wagner, Paul Butler

**Paper 237e:** Holographic Characterization of Three-Dimensional Velocity Fields in Viscoelastic Flows — **Siddhartha Gupta**, Siva A. Vanapalli

**Paper 237g:** Flow Visualization of Closed Loop Pulsating Heat Pipe (CLPHP) Charged with Olive Oil for High Temperature Applications — **Manoj Kumar**, Arup Kumar Das, Prasanta Kumar Das

**Paper 237w:** Characterization of Bubble Dynamics and Local Gas Holdup in a Cylindrical Airlift Photobioreactor during Microalgae Culturing — **Aastha Ojha**, Laith Sabri, Muthanna H. Al-Dahhan

**Paper 237x:** Influence of Heat Exchanging Dense Internals on the Flow Dynamics Parameters in Bubble Column with and without Internals via Radioactive Particle Tracking (RPT) Technique — **Abbas Sultan**, Laith Sabri, Muthanna H. Al-Dahhan

**Paper 237y:** Local Hydrodynamics Characteristics of Cylindrical Split Airlift Reactor via Radioactive Particle Tracking (RPT) Technique — **Laith Sabri**, Abbas Sultan, Muthanna H. Al-Dahhan

**Paper 237h:** A VoF-LPT Solver for 3D Numerical Simulation of Aerated Slug Flow and Closure Law Development — **Stefan Radl**, Arianna Bonzanini, Pietro Poesio

**Paper 237j:** Analysis of the Effect of Wetting Film on Two-Phase Flow in a Micromodel Porous Pattern: A CFD Approach — **Ali Nabizadeh**, Hossein Hassanzadeh, Jalal Fahimpour, Mostafa K. Moraveji

**Paper 237k:** Computational Fluid Dynamics Simulation of Lignocellulosic Biomass Transport in a Compression-Screw Feeder — **Mohammad J. Rahimi**, Hariswaran Sitaraman, James J. Lischeske, David A. Sievers, Erik Kuhn, Jonathan J. Stickel

**Paper 237l:** Droplet Generation in Two Phase Liquid-Liquid Flow Systems in Millichannels – Effect of Phase Inlet Orientation and Reactant Mass Flux — **Alex Koshy**, Gargi Das, Subhabrata Ray

**Paper 237m:** A New Perspective on the Wetting of a Solid Surface By the Drops of an Emulsion — **Arun Ramchandran**, Suraj Borkar

**Paper 237n:** Thin Free Liquid Film Stability in Various Interaction Regimes Arising Due to Surface Active Agents — **Anjishnu Choudhury**, Paidi Venkatesh Kumar, Harish N. Dixit, Sreeram K. Kalpathy

**Paper 237o:** Free Surface Flows and Extensional Rheology of Polymer Solutions — **Jelena Dinic**, Leidy N. Jimenez, Vivek Sharma

**Paper 237p:** Rheology of Silica Nanoparticle Dispersions Under High Shear — **Ehsan Akbari Fakhrahadi**, Caleb Morehart, Matthew Liberatore

**Paper 237q:** Numerical and Recursion Solution of the Shear Stress of Biological Fluids in Rectangular and Cylindrical Capillary Vessels — **Mathias A. Oyanader**, Mario Oyanader

**Paper 237r:** Following the Hemo-Rheology of Cardiac Surgery Patients - RBC Aggregation and Blood Viscoelasticity — **Yeng-Long Chen**, Yi-Fan Wu, Po-Hsun Hsu

**Paper 237s:** Multifluid Modelling Approaches for the Numerical Investigation of Liquid-Solid Suspensions: Limitations and Challenges — **Rashid Jamshidi**, Giovanni Meridiano, Panagiota Angeli, Luca Mazzei

**Paper 237t:** Flow Patterns of Gas-Liquid Cocurrent Downward Flow through an Orifice Plate — **Min Qiao**, Weixing Huang, Chaojun Deng, Junfeng Li, Yunxiang Xue

**Paper 237u:** Fabrication of Solid in Water in Oil (S/W/O) Compound Droplets Via a Microfluidic T-Junction Device — **Dawei Pan**, Meifang Liu, Weixing Huang, Bo Li

**(238) Process Scale-up Techniques Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 336

Rob Nunley, Co-Chair  
Jayachandran Devaraj, Co-Chair

**Sponsored by:** Pilot Plants

**3:30 Break**

**4:00 Paper 238b:** Practical Methods for Process Scale-up — **Moshe Bentolila**

**4:30 Paper 238c:** Commercializing the Production of 1,3 Butadiene through the Production of 2,3 Butanediol Using Intrexon's Natural Gas-to-Liquids Platform — **Bryan Yeh**, Christina Bodarky, Stephen Kasprzyk, John Burgess

**5:00 Paper 238d:** Comparison of Distillation Strategies, Optimization and Scale-up for an Industrial Process Based on Mechanistic Modelling — **Rui Pina Campos**, Filipe Ataíde, João Sardinha, António Henriques

**(239) PSA/TSA**

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 305

Roger D. Whitley, Chair  
Federico Brandani, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**3:30 Paper 239a:** Experimental Investigation and Simulation of the CO<sub>2</sub> Removal with Indirectly Heated and Cooled Adsorbents — **Thomas Ried**, Gabriel Salazar Duarte, Christian Voss, Olaf Hinrichsen

**3:55 Paper 239b:** Structured Adsorbent Pressure Temperature Swing Adsorption Cycles for Metabolic CO<sub>2</sub> Removal from Spacecraft Cabins — **Armin D. Ebner**, Ryan T. Sanders, James C. Knox, James A. Ritter

**4:20 Paper 239c:** Comparison of Different Intensified Alternatives for the Downstream Separation in the OCM Process — **Cristian C. Rodriguez**, Alvaro Orjuela, Miguel Santaella, Jens-Uwe Repke, Erik Esche, Hamid Godini, Alberto Penteado, Hector D. Diaz Ortiz

**4:45 Paper 239d:** Improved Kinetic Pressure Swing Adsorption Process — **Shubhra J. Bhadra**, Roger D. Whitley, Erdem Arslan, Dingjun Wu

**5:10 Paper 239e:** Enrichment of Low Concentration  $\text{CH}_4/\text{N}_2$  Mixture By Adsorption Process with Displacement Chromatography Technology — **Ying Yang, Kai Lu, Donglei Qu, Ping Li, Jianguo Yu**

**5:35 Paper 239f:** Simulation Study of Concentrating High Purity  $\text{CO}_2$  from Syngas after Oxy-Fuel Combustion By Pressure Swing Adsorption Process — **Cheng-tung Chou, Wei-Yu Chen, Tien-Lin Wu, Hong-Sung Yang**

**(240) Rational Catalyst Design III**  
**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 403

Kenneth L. Roberts, Chair  
Zhenglong Li, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 240a:** Elucidating Mechanisms of Plasmon Decay in Multimetallic Nanostructures for the Rational Design of Plasmonic Photocatalysts — **Steven Chavez, Umar Aslam, Suljo Linic**

**3:50 Paper 240b:** Computational Investigation of Transition Metal Alloying Effects on the Structure and Enhanced Stability of Pt-Ni Nanoparticles — **Liang Cao, Tim Mueller**

**4:10 Paper 240c:** Design of Non-Stoichiometric Mixed Metal Oxides As Electrocatalysts for Oxygen Reduction — **Xiang-Kui Gu, John Carl A. Camayang, Samji Samira, Ayad Nacy, Eranda Nikolla**

**4:30 Paper 240d:** Oxide Heterostructure Systems for Oxygen Evolution Reaction - Activation of  $\text{SrTiO}_3$  with Subsurface  $\text{SrRuO}_3$  — **Aleksandra Vojvodic**

**4:50 Paper 240e:** Overcoming Site Heterogeneity in Search of Metal Nanocatalysts for Oxygen Reduction — **Siwen Wang, Noushin Omidvar, Emily Marx, Hongliang Xin**

**5:10 Paper 240f:** Active Learning across Intermetallics Guides Discovery of Electrocatalysts for Carbon Dioxide Reduction and Hydrogen Evolution — **Kevin Tran, Zachary Ulissi**

**5:30 Paper 240g:** Design of Optimal Metallic Surface Reconstructions for Heterogeneous Catalysis — **Christopher L. Hanselman, Wen Zhong, Kevin Tran, Zachary Ulissi, Chrysanthos E. Gounaris**

**(241) Reaction Chemistry and Engineering II**

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 404

Sarsani Sagar, Chair  
Eric G. Moschetta, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 241a:** Continuous Hydrogen Generation for PEM Fuel Cell Vehicles Using Catalytic Decomposition of Hydrous Hydrazine: Experiments and Model — **Wooram Kang, Arvind Varma**

**3:51 Paper 241b:** Initial Rate Kinetics of Pyrene Polymerization Catalyzed with  $\text{AlCl}_3$  — **William Lamie, Mark C. Thies, David A. Bruce**

**4:12 Paper 241c:** Unravelling the Catalytic Effect of Naturally Occurring Inorganics on Biomass Pyrolysis Chemistry: A Combined Experimental and DFT Study — **Jyotsna S. Arora, Khurshed B. Ansari, Paul J. Dauenhauer, Samir H. Mushrif**

**4:33 Paper 241d:** Effects of Morphology and Dopants on the  $\text{CO}_2$  Capacity of Nanofibrous Calcium-Oxide Based Materials for Sorption-Enhanced Steam Methane Reforming — **Dante Simonetti, Luke Minardi, Faisal H. Alshafei, Zubin Mishra**

**4:54 Paper 241e:** A Strategy for Developing Structure-Based Kinetic Model for Hydrodesulfurization Reactor Under Petroleomics Concept — **Thuy T. H. Nguyen, Sho Kataoka, Yuki Takahashi, Koji Tsuji, Ryuzo Tanaka**

**5:15 Paper 241f:** Estimating Kinetic Parameters from Batch Data: Breaking Correlations Using Mixed-Effects Models — **Daniel W. Trahan, Fabio D'Ottaviano, Michael Ignatowich, Daniel A. Hickman**

**5:36 Paper 241g:** Triethyl and Tributyl Citrate Production from Dicalcium Citrate Salt: Esterification Kinetics — **Andres F. Cabeza, Alvaro Orjuela**

**(242) Risk Reduction in - and Implementation of - Process & Technology Development**

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 334

John Peragine, Chair  
William Hollar, Co-Chair

**Sponsored by:** Technology Transfer and Manufacturing

**3:30 Paper 242a:** Development of Mobile Decontamination Equipment for Hazardous Materials — **Jinwoo Park, Hyungjoon Yoon, Sunghyun Cho, Myeongseok Lee, Changyun Choi, Myungjae Seo, Il Moon**

**3:55 Paper 242b:** Process Optimization to Reduce Urea Plant Startup Failure Rate and Ammonia Pollution — **Naveed Raza, Ali Ayub**

**4:20 Paper 242c:** Launching Clinical Antisense Oligonucleotide Manufacturing Capability in a Biologics Company — **Sheron Branham, Jesse Faber**

**4:45 Break**

**5:10 Paper 242f:** Reaction Engineering for Energetic Material Synthesis — **Eric Gauthier, Kelley Caflin**

**(243) Solar Energy for Power Generation and Chemical Processing II**

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 324

Alexandre Yokochi, Chair  
Nick AuYeung, Co-Chair  
Wojciech Lipinski, Co-Chair  
Peter Kreider, Co-Chair

**Sponsored by:** Solar Energy for Power Generation and Chemical Processing

**3:30 Paper 243a:** Theoretical and experimental investigation of effective solar mixed reforming for a less carbon intensive production of methanol — **Henrik von Storch, Patrick Hilger, Carlos Rendon, Zahra Mahdi, Nicolas Overbeck, Lamark de Oliveira, Christian Sattler, Martin Roeb**

**3:48 Paper 243b:** Integrated Solar-Thermochemical Reactor/ Gas Recuperator for Upgrading Light Hydrocarbons — **Lucas Freiberg, Fuqiong Lei, Matthew Coblyn, Nick AuYeung, Goran N. Jovanovic, Alexandre Yokochi**

**4:06 Paper 243c:** Solar Thermochemical Hydrogen/Syngas Production from Methane and/or Biogas in the Presence of Non-stoichiometric Solid Oxide Carriers — **Elena Galvez, Patrick Da Costa, Romain Guibert**

**4:24 Paper 243d:** Dynamic Performance of Fischer-Tropsch Liquid Fuel Production from Solar-Assisted Supercritical Water Gasification of Algae — **Alireza Rahbari, Ali Shirazi, Mahesh Venkataraman, John Pye**

**4:42 Paper 243e:** Solar Thermal Ethane Cracking — **Fuqiong Lei, Yige Wang, Lucas Freiberg, Ian Reddick, Alexandre Yokochi, Goran Jovanovic, Nick AuYeung**

**5:00 Paper 243f:** Scope of zero-carbon metal production: State-of-the-art and future prospects — **Mahesh Venkataraman, Alireza Rahbari, Wojciech Lipinski, John Pye**

**5:18 Paper 243g:** Green Steam Initiative: Novel and Cost Effective Parabolic Trough Collector System — **Deepankar Biswas**

**5:36 Paper 243h:** Stochastic Optimization to Reduce Cost of Energy for Parabolic Trough Solar Power Plant for Different Weather Conditions — **Adarsh Vaderobli, Urmila M. Diwekar**

**(244) Surface Engineered and Responsive Membranes**

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 301

Ayşe Asatekin, Co-Chair  
Dona Foster, Co-Chair  
Ranil Wickramasinghe, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 244a:** Patterning Various Commercial Nanofiltration and Reverse Osmosis Membranes — **Steven T. Weinman, Eric M. Fierce, Scott M. Husson**

**3:48 Paper 244b:** Membrane Surface Modification Using Acrylate- and Thiol-Containing Zwitterionic Materials Via Bio-Adhesive Polydopamine — **Nima Shakhkaramipour, Chong Cheng, Haiping Lin**

**4:06 Break**

**4:24 Paper 244d:** High-Flux, High Capacity Adsorptive Membranes Based on Polysulfone and Block Polymer Composites — **Yizhou Zhang, William A. Phillip**

**4:42 Paper 244e:** High Performance Electrospun Nanofiber Membranes for Protein Purifications — **Shu-Ting Chen, S. Ranil Wickramasinghe, Xianghong Qian**

**5:00 Paper 244f:** Pnipam Functionalized Temperature Responsive Membranes and Pollutant Adsorption — **Anthony Saad, Hongyi Wan, Dibakar Bhattacharyya**

**5:18 Paper 376ae:** PVDF Membrane Pore Functionalization Approaches with Applications to Pollutant Remediation — **Mohammad Saiful Islam, Hongyi Wan, Dibakar Bhattacharyya**

#### (245) Thermodynamic and Transport Properties Under Pressure

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 306

Kenneth M. Benjamin, Chair  
Christopher L. Kitchens, Co-Chair

**Sponsored by:** High Pressure

**3:30 Paper 245a:** Measurements and Modeling of the Density and Viscosity of Rocket Propellant RP-2 at Temperatures to 300 °C and Pressures to 100 Mpa — **Rajendar R. Mallepally, Babatunde A. Bamgbade, Mark A. McHugh, Hseen O. Baled, Robert M. Enick, Matthew C. Billingsley**

**3:54 Paper 245b:** Speed of Sound and Density of (Carbon Dioxide + Nonane) and (Carbon Dioxide + Methylbenzene) at Temperatures between (283 and 473) K and Pressures up to 390 Mpa — **J. P. Martin Trusler, Weparn J. Tay**

**4:18 Paper 245c:** Density and Viscosity of Star/Linear Polystyrene + Toluene Mixtures at Temperatures to 523 K and Pressures to 200 Mpa: Experiments and Modeling — **Rajendar R. Mallepally, Babatunde A. Bamgbade, Matthew S. Newkirk, Mark A. McHugh**

**4:42 Paper 245d:** High-Pressure, High-Temperature Interfacial Tension of n-Alkane + Nitrogen Mixtures — **Aaron J. Rowane, Rajendar R. Mallepally, Mark A. McHugh, Ashutosh Gupta, Manolis Gavaises**

**5:06 Paper 245e:** Effect of CO<sub>2</sub>-Philic Additives and Co-Blow Agents on CO<sub>2</sub> Diffusion in Polystyrene Microcellular Foaming — **Wei Qiang**

**5:30 Paper 245f:** Calculation on the Heat Transfer Correlations and Simulation Verification for Typical LNG Open Rack Vaporizer — **He Cheng, Yonglin Ju, Yunzhun Fu**

#### (246) World Cafe: Food-Energy-Water Nexus (Invited Talks and Panel Discussion)

**Monday, Oct 29, 3:30 PM**

David L. Lawrence Convention Center, 317

Leslie M. Shor, Chair  
Nada Assaf-Anid, Co-Chair  
Dale Keairns, Co-Chair  
JoAnn S. Lighty, Co-Chair

**Sponsored by:** The Food-Energy-Water Nexus

**3:30** Welcoming Remarks

**3:35 Paper 246a:** Introductory Remarks by Panelist Jack Starr — **Jack Starr**

**3:45 Paper 246b:** The Intersection of Energy-Water-Food for Electric Power Generation — **Briggs White**

**3:55 Paper 246c:** Introductory Remarks by Panelist Richard Darton — **Richard C. Darton**

**4:05 Paper 246d:** Introductory Remarks by Panelist Anton Middelberg — **Anton P. J. Middelberg**

**4:15 Paper 246e:** Introductory Remarks by Panelist Matthew Stuber — **Matthew D. Stuber**

**4:25** Panel Discussion

#### (247) Theory, Modeling, and Simulation of Nuclear Chemical Processes I

**Monday, Oct 29, 4:15 PM**

David L. Lawrence Convention Center, 327

Valmor F. de Almeida, Chair  
Candido Pereira, Co-Chair

**Sponsored by:** Nuclear Engineering Division

**4:15 Paper 247a:** Mobile Boration System — **Ryan Vanston, Matthew Swartz, John Lojek**

**4:36 Paper 247b:** Analysis of Air Oxidation of Plutonium Metal — **James E. Laurinat**

**4:57 Paper 247c:** Study of Tritium Solubility and Diffusivity in Lithium Aluminate and Lithium Zirconate Pellets in Tpbir Using First Principle Density Functional Theory — **Hari Paudel, Yueh-Lin Lee, Yuhua Duan**

**5:18 Paper 247d:** Analysis of Helium Segregation on Surfaces of Plasma-Exposed Tungsten — **Lin Hu, Asanka Weerasinghe, Karl D. Hammond, Brian D. Wirth, Dimitrios Maroudas**

**5:39 Paper 247e:** Nonlinear Dynamics of Bubble Collapse — **Jyoti Bhati, Swapan Paruya, S. Pushpavanam**

#### (248) Marketing is Not Bragging: How to Articulate Your Value to Advance Your Career

**Monday, Oct 29, 4:45 PM**

David L. Lawrence Convention Center, 330

April Grasso, Chair

**Sponsored by:** Publication Committee

**4:45 Paper 248a:** Marketing is Not Bragging: How to Articulate Your Value to Advance Your Career — **Alaina Levine**

#### (249) D.I.C. Wang Award Lecture

**Monday, Oct 29, 6:00 PM**

Westin Convention Center, Allegheny Grand Ballroom I

Georges Belfort, Chair

**Sponsored by:** Awards Committee

**6:00 Paper 249a:** Lessons from a Life in Biopharma — **John G. Auninš**

#### (250) Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony

**Monday, Oct 29, 6:30 PM**

Westin Convention Center, Allegheny Grand Ballroom II

Jonathan McMullen, Chair  
John Lepore, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

#### (251) Advanced Problem Solving in the Chemical Industry III

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 407

Zdravko Stefanov, Chair

**Sponsored by:** Young Professionals Committee (YPC)

#### (252) Advancements in Polymers and Amorphous Solids for Pharmaceutical Process Development

**Tuesday, Oct 30, 8:00 AM**

Westin Convention Center, Fayette

Blair Kathryn Brettmann, Chair  
Pavithra Sundararajan, Co-Chair  
Steven J. Brenek, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**8:00 Paper 252a:** Synthetic and Compositional Control of Multicomponent Copolymers to Promote Drug Solubility and Bioavailability — **Theresa M. Reineke**

**8:40 Paper 252b:** Nanocellulose Gels As a Flexible, High Surface Area Material for Crystallizing Pharmaceuticals — **Blair Kathryn Brettmann**

**8:58 Paper 252c:** Controlling the Particle Morphology of Spray Dried Poly(methacrylic acid-co-methyl methacrylate) (Eudragit L100) Polymer — **Kimberly B. Shepard, Michael Morgen**

**9:16 Paper 252d:** Application of Fundamental Relationships and Models to Predict Spray-Dried Dispersion Particle Size — **John Baumann, Alyssa Ekdahl, Chris Craig**

**9:34 Paper 252e:** Improving Spray Drying Processing through Modeling and Characterization — **Pavithra Sundararajan**

**9:52 Paper 252f:** Mechanistic Approach to Predict Amorphous Solid Dispersion Thermal Degradation in Spray Drying Processes — **Gonçalo Poelras, Tiago Porfirio, Clara Sá Couto, João Pereira, Rui C. Silva, Iris Duarte, Maria Diná Afonso, João Vicente**

**10:10 Paper 252g:** Downstream Processing of a Ternary Amorphous Solid Dispersion: The Impacts of Spray Drying and Hot Melt Extrusion on Powder Flow, Compression and Dissolution — **Mark Davis, Catherine Kelly, Gavin Walker**

#### (253) Advances in Deterministic Global Optimization

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 409

Selen Cremaschi, Chair  
Kamil A. Khan, Co-Chair

**Sponsored by:** Computers in Operations and Information Processing

**8:00 Paper 253a:** Enhancing Relaxations for Nonconvex Mixed-Integer Quadratically-Constrained Quadratic Programs — **Carlos Nohra, Aida Khajavirad, Nick Sahinidis**

**8:19 Paper 253b:** Advances in Decomposition Strategies for Non-Convex Nonlinear Programs — **Jose S. Rodriguez, Bethany Nicholson, Carl D. Laird, Victor M. Zavala**

**8:38 Paper 253c:** Online Generation Via Offline Selection of Strong Linear Cuts from a Semidefinite Programming Relaxation — **Radu Baltean-Lugojan, Pierre Bonami, Andrea Tramontani, Ruth Misener**



**8:57 Paper 253d:** New Underestimator and Branching Scheme for the Global Optimization of General Nonconvex Problems — *Ishan Bajaj, M. M. Faruque Hasan*

**9:16 Paper 253e:** On Piecewise Under- and over-Estimators of Fractional Terms — *Radhakrishna Tumbalam Gooty, Rakesh Agrawal, Mohit Tawarmalani*

**9:35 Paper 253f:** Quadratic Underestimators of Differentiable McCormick Relaxations for Deterministic Global Optimization — *Matthew Wilhelm, Matthew D. Stuber*

**9:54 Paper 253g:** A Novel Branching Scheme for Problems with Reverse Convex Quadratic Constraints and Its Application to Packing Problems — *Akang Wang, Christopher L. Hanselman, Chrysanthos E. Gounaris*

**10:13 Paper 253h:** Subtangent-Based Approaches for Optimization of Parametric Process Systems — *Kamil A. Khan*

#### (254) Advances in Enzymatic Catalysis I

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 405

Heather Mayes, Chair  
Andrew J Adamczyk, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 254a:** Machine Learning Approaches for Enzyme Engineering — *Sanjan T.P. Gupta, Evan Glasgow, Brian G. Fox, Parmeswaran Ramanathan, Jennifer L. Reed*

**8:30 Paper 254b:** Simulating the Mechanistic Pathway of Transglycosylation Via a Mutant Glycoside Hydrolase — *Tucker Burgin, Heather Mayes*

**8:50 Paper 254c:** Engineering a Multifunctional Family 5 Glycosyl Hydrolase into a Transglycosidase — *Chandrakanth Bandi, Antonio Goncalves, Shishir Chundawat*

**9:10 Paper 254d:** Computational Insights into the Catalytic Function of Processive Cellulases — *Brandon C. Knott, Joshua Vermaas, Jerry Ståhlberg, Gregg T. Beckham, Michael F. Crowley*

**9:40 Paper 254e:** Enhanced Lipase-Catalyzed Hydrolysis and Modification of Fats and Oils — *Akash Anand*

**10:00 Paper 254f:** Activity Improvement of D-Psicose-3-Epimerase from *Agrobacterium tumefaciens* CGMCC 1.1488 By Site-Directed Mutagenesis — *Xiaoyan Chen, Shijie Liu, Zhenhong Yuan, Jingliang Xu*

#### (255) Advances in Membrane Technologies for Food and Bioprocessing

**Tuesday, Oct 30, 8:00 AM**  
Westin Convention Center, Westmoreland East

Gaohong He, Chair  
Michelle C. Almendrala, Co-Chair  
Xiaobin Jiang, Co-Chair

**Sponsored by:** Food

**8:00 Paper 255a:** Functionalized Mesh Materials for Listeria Control in Dairy Applications — *Stephen Ritchie*

**8:18 Paper 255b:** Electrospun Carbon Nanotube/Sulfonated Poly (ether ether ketone) Proton Conductive Membranes for Vanadium Redox Flow Battery — *Xuemei Wu, Fujun Cui, Jie Li, Daishuang Zhang, Sangshan Peng, Gaohong He*

**8:36 Paper 255c:** Directing Filtration to Narrow Molecular Weight Distribution of Oligodextran in an Enzymatic Membrane Reactor — *Ziran Su, Jianquan Luo, Yinhua Wan*

**8:54 Paper 255d:** A Compact Double Crosslinking Technique for High Performance Solvent Resistant Nanofiltration Membrane Fabrication — *Akbar Asadi Tashvigh, Yingnan Feng, Lin Luo, Neal Tai-Shung Chung, Martin Weber, Christian Maletzko*

**9:12 Paper 255e:** One Step Co-Sintering Process for Low-Cost Fly Ash Based Ceramic Microfiltration Membrane — *Dong Zou, Minghui Qiu, Enrico Drioli, Yiqun Fan*

**9:30 Paper 255f:** Ultrafiltration Effect on the Physicochemical Properties of Coconut Water Using Polysulfone Hollow Fiber Membrane — *Michelle C. Almendrala, Nerio Gacutan Jr., Shaira Celocia*

**9:48 Paper 255g:** Decoloration of Molasses By Ultrafiltration and Nanofiltration: Understanding the Mechanisms of High Sucrose Retention — *Yinhua Wan, Jianquan Luo, Shiwei Guo*

#### (256) Advances in Metabolic Engineering: Biosynthetic Pathway Engineering and Enzymatic Conversion

**Tuesday, Oct 30, 8:00 AM**  
Westin Convention Center, Westmoreland West-Central

Ryan Summers, Chair  
Kevin V. Solomon, Co-Chair  
Mark Blenner, Co-Chair

**Sponsored by:** Bioengineering

**8:00 Paper 256a:** A Novel Two Step Pathway for Isoprenoid Synthesis — *Alkiviadis Chatzivasileiou, Valerie Ward, Steven Edgar, Gregory Stephanopoulos*

**8:18 Paper 256b:** Engineering Cellulolytic Bacterium *Clostridium Thermocellum* to Co-Ferment Cellulose- and Hemicellulose-Derived Sugars Simultaneously — *Luis H. Reyes, Wei Xiong, William Michener, Pin-Ching Maness, Katherine J. Chou*

**8:36 Paper 256c:** Animal-Free Chondroitin Sulfate Production through Protein Engineering and Metabolic Engineering Strategies — *Asher J. Williams, Wenqin He, Mattheos A. G. Koffas, Robert J. Linhardt*

**8:54 Paper 256d:** Metabolic Engineering of the High Native Capacity of *Kluyveromyces Marxianus* to Synthesize Ethyl Acetate — *Ann-Kathrin Löbs, Cory Schwartz, Sarah Thorwall, Ian Wheeldon*

**9:12 Paper 256e:** Engineering *Saccharomyces Cerevisiae* for Production of Iridoids — *John M. Billingsley, Yi Tang*

**9:30 Paper 256f:** Genetic Refactoring for the Implementation of Formaldehyde-Based Regulation in *Escherichia coli* for Synthetic Methylothrophy — *Julia R. Rohlfhill, Robert K. Bennett, Eleftherios Terry Papoutsakis*

**9:48 Paper 256g:** Engineering Inhibitor Tolerance — *Laura Jarboe*

**(257) Advances in Process Control I**  
**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 408

Fernando V. Lima, Chair  
Ali Mesbah, Co-Chair

**Sponsored by:** Systems and Process Control

**8:00 Paper 257a:** Perspectives on the Control of Advanced Manufacturing Systems — *Joel Paulson, Eranda Harinath, Lucas Foguth, Richard D. Braatz*

**8:19 Paper 257b:** Investigating the Impacts of Time-Varying Operation on Equipment Fidelity — *Matthew Wegener, Helen Durand*

**8:38 Paper 257c:** Generalized Chaos Expansions with Arbitrary Multivariate Probability Measures: Applications in Closed-Loop Performance Verification for Stochastic Dynamic Systems — *Joel Paulson, Ali Mesbah*

**8:57 Paper 257d:** Constrained Control Lyapunov Function Construction Via Approximation of Static Hamilton-Jacobi-Bellman Equations — *Tyler Homer, Prashant Mhaskar*

**9:16 Paper 257e:** On Multiparametric/Explicit NMPC for Quadratically Constrained Problems — *Nikolaos A. Diangelakis, Iosif S. Pappas, Efstratios N. Pistikopoulos*

**9:35 Paper 257f:** Explicit Model Predictive Control Using Nonlinear Intrinsic Variables — *Robert J. Lovelett, Felix Dietrich, David Sroczynski, Ioannis G. Kevrekidis*

**9:54 Paper 257g:** Closest Feasible Point Invariance: A New System Property to Characterize Input-Constrained Systems — *Masoud Soroush*

**10:13 Paper 257h:** Securing Process Control Systems Using Dynamic Watermarking — *Joseph Sangil Kwon, Bharadwaj Satchidanandan, Woo-Hyun Ko, Jaewon Kim, Abhinav Narasingam, P. R. Kumar*

#### (258) Advances in Process Intensification

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 335

Chongwei Xiao, Chair  
Robert S. Huss, Co-Chair

**Sponsored by:** Process Intensification & Microprocess Engineering

**8:00 Paper 258a:** Development and Evaluation of Oxidative Dehydrogenation Technology for Production of Light Olefins — *Gennaro J. Maffia, Anne Gaffney, Aaron Beinstein*

**8:21 Paper 258b:** Process Intensification through Membrane Separation of Olefins and Paraffins — *Hannah Murnen, Sudip Majumdar, William Charlton, Ken Loprete, Ning Shangguan, Affiq Zulkifli, Kenneth J. Pennisi*

**8:42 Paper 258c:** Evaluation of Novel Mixing and Separation Apparatus for Liquid-Liquid Extraction — *Arjun Kumar Pukkella, Raviraju Vysyaraju, Sivakumar Subramanian*



**9:03 Paper 258d:** 2D Optimization of Fixed-Bed Reactors: Additional Degrees of Freedom for the Reactor Design to Increase Efficiency — **Alexander Pietschak**, Hannsjörg Freund

**9:24 Paper 258e:** On-Sun Demonstration of Continuous Redox Driven Solar Thermochemical Hydrogen Production — **Amanda Hoskins**, Samantha L. Millican, Caitlin Czernik, Judy Netter, Alan W. Weimer

**9:45 Paper 258f:** The Mechanism Investigation for Process Intensification of the Esterification Reaction By Microwave Irradiation — **Xin Gao**, Hong Li, Ying Meng

**10:06 Paper 258g:** Process Intensification Via Batch-to-Continuous Transition in the Production of Lubricants: Acquisition of Robust Reaction Kinetics — **Nasser Al Azri**, Edmund Sam-Gyandoh, Samuel Batchelder, Zibo Zhen, Hari C. Mantripragada, Robert M. Enick, Cliff Kowall, Götz Vesper

#### (259) Alternative Fuels including Biofuels, Hydrogen, Renewable Hydrogen, and Syngas

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 324

Haider Al-Rubaye, Chair

**Sponsored by:** Transport and Energy Processes

**8:00 Paper 259a:** Modelling of Multiphase Behavior of Biodiesel Transesterification Operating Below Critical Conditions Using CO<sub>2</sub> as a Co-solvent with PC-SAFT EoS — **Gianfranco Rodriguez**, Eric J. Beckman

**8:22 Paper 259b:** High Pressure Hydrogen Generation and Simultaneous Carbon Dioxide Separation with Chemical Looping Hydrogen — **Robert Zacharias**, Sebastian Bock, Viktor Hacker

**8:44 Paper 259c:** Renewable Transport Fuels, Heat and Electricity from Miscanthus: Optimisation for Design, Planning and Operation of Sustainable Value Chains — **Ryan Grubb**, Sheila Samsatli

**9:06 Paper 259d:** Gasification of Glucose in the Reactor CREC-Riser Simulator: Stable Ni-(La or Ce)/g-Alumina Catalysts and Effect of Reaction Time and Steam/Glucose — **Benito Serrano Sr.**, Adriana Sanchez, Daniel Gibrán Gonzalez Castañeda Sr., Ivan Cruz Reyes, Alan Ruben Calzada Hernandez Sr., Hugo de Lasa

**9:28 Paper 259e:** Effect of Stirring on the Hydrate Formation Rate for Natural Gas Storage and Transportation Perspective — **M. Fahed Qureshi**, Majeda Khraisheh, Tausif Altamash, M.a Saleh

**9:50 Paper 259f:** MgO/Mg Based Solar Driven CH<sub>4</sub> Reforming and H<sub>2</sub>O Splitting Process — **Rahul Bhosale**, Gorakshnath Takalkar

**10:12 Paper 259g:** Solid-Liquid and Vapor-Liquid Equilibria of BTEX Compounds in Methane and Ethane Mixtures at LNG Conditions — **Saif ZS. Al Ghafri**, Arman Siahvashi, Eric F. May

#### (260) Area Plenary: Adsorption and Ion Exchange II: Fundamentals and Applications

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 305

Peter I. Ravikovitch, Chair  
Stefano Brandani, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**8:00 Paper 260a:** On the Use of the Dual Process Langmuir Model for Gas Mixture Components That Exhibit Single Process or Linear Isotherms — **James A. Ritter**, Kathryn C Bullmiller, Lutfi Erden, Armin D. Ebner

**8:20 Paper 260b:** The Rigid Adsorbent Lattice Fluid Model: A New Thermodynamic Framework for Multicomponent Adsorption — **Stefano Brandani**

**8:40 Paper 260c:** Constant-Pattern Design Method for Separating Ternary Mixtures of Rare Earth Elements Using Ligand-Assisted Displacement Chromatography — **Hoon Choi**, David M. Harvey, Yi Ding, Nien-Hwa Linda Wang

**9:00 Paper 260d:** The Effect of Aluminum Ordering on Carbon Dioxide Adsorption in Zeolites — **John Findley**, Peter I. Ravikovitch, David S. Sholl

**9:20 Paper 260e:** Ethane Diffusion in a Mixed Linker ZIF-7-8 By Pulsed Field Gradient NMR in Combination with a Single Crystal IR Microscopy — **Samuel Berens**, Christian Chmelik, Jörg Kärger, Febrin Hillman, Hae-Kwon Jeong, Sergey Vasenkov

**9:40 Paper 260f:** Evaluation of Carbon Monoliths for CO<sub>2</sub> Separation — **Ana Martin-Calvo**, Brieuc Veroughstraete, Stijn Van der Perre, Joeri Denayer

**10:00 Paper 260g:** A Critical Review on the Merits and Fallacies of Adsorption Kinetics Models — **Vassilis J. Inglezakis**, Marios Fyrillas

#### (261) Area Plenary: Bionanotechnology (Invited Talks)

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 311

Kathryn A. Whitehead, Chair  
Millicent Sullivan, Co-Chair  
Lorraine Leon, Co-Chair

**Sponsored by:** Bionanotechnology

**8:00 Paper 261a:** Design and Engineering of Biohybrid Materials for Organic Electronics: From Supramolecular Assembly to Single Molecule Charge Transport — **Charles M. Schroeder**

**8:50 Paper 261b:** Lipid-like Materials for RNA Delivery: Predicting In Vivo Efficacy — **Kathryn A. Whitehead**

**9:40 Paper 261c:** Photoresponsive Nanomaterials in Tissue Repair and Radiotherapy — **Kaushal Rege**

#### (262) Area 8E Graduate Student Award Finalists (Sponsored by JVST)

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 330

Aaron T. Fafarman, Chair

**Sponsored by:** Electronics and Photonics

**8:00 Paper 262a:** Rational Surface Modification of Two-Dimensional Black Phosphorus: Insights from First-Principles Calculations — **Tong Mou**, Bin Wang

**8:20 Paper 262b:** Reviving Pyrite FeS<sub>2</sub> as a Photovoltaic Material — **Bryan Voigt**, Jeff Walter, Xin Zhang, Debmalaya Ray, Michael Manno, Laura Gagliardi, Eray S. Aydi, Chris Leighton

**8:40 Paper 262c:** Evaluating Novel Semiconducting Materials for Photovoltaic Applications: A Case Study of Copper Arsenic Sulfide (Cu<sub>3</sub>AsS<sub>4</sub>) — **Scott McClary**, Weiwei Meng, Xinxing Yin, Joseph Andler, Siming Li, Louis Schroeder, Jason B. Baxter, Carol Handwerker, Yanfa Yan, Rakesh Agrawal

**9:00 Paper 262d:** Molecular Design of Cooperative Transition for Shape Memory Electronics — **Hyunjoong Chung**, Ying Diao

**9:20 Paper 262e:** Long-Time Molecular Simulations for Linking Organic Semiconductor Morphologies to Carrier Mobilities — **Michael Henry**, Evan Miller, Matthew Jones, Eric Jankowski

**9:40 Paper 262f:** Structure and Composition Tuning of Bismuth-Halide Perovskites — **Rainie D. Nelson**, Matthew G. Panthani

**10:00 Paper 262g:** Modeling of Quantum Dot Pattern Formation on Pit-Patterned Semiconductor Substrates — **Ashish Kumar**, Lin Du, Chao-Shou Chen, Dimitrios Maroudas

#### (263) Biofuels Production: Design, Simulation, and Economic Analysis

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 316

Ana I. Torres, Chair  
Ramalingam Subramaniam, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**8:00 Paper 263a:** Process Intensification of Algae Oil Extraction to Biodiesel — **Geetanjali Yadav**, Warren D. Seider, Lindsay Soh, Julie Zimmerman, Leonard Fabiano

**8:21 Paper 263b:** Regional Techno-Economic (TEA) Analysis of the Pyrolysis-Bioenergy-Biochar Pathway for Carbon-Negative Energy — **Wenqin Li**, Jerome Dumortier, Hamze Dokoohaki, Fernando E. Miguez, Mark Mba Wright, Robert C. Brown, David Laird

**8:42 Paper 263c:** Modelling Hydrogen Production Via Combined Hydrothermal Liquefaction of Macroalgae *Saccharina japonica* and Hydrothermal Gasification of Aqueous Product Using Aspen Plus® — **Haider Niaz**, Boris Brigljevic, J. Jay Liu

**9:03 Paper 263d:** Process Simulation and Experimental Investigation of Biofuel Production in a High RATE Anaerobic Digestion Process — **Haider Al-Rubaye**, Joseph D. Smith, Manohar Manchenahalli



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AIChEvents app.

**(264) Biomaterials for Drug Delivery****Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 328

Srivatsan Kidambi, Co-Chair  
Timothy Brenza, Co-Chair  
Stephanie Christau, Co-Chair**Sponsored by:** Biomaterials**8:00 Paper 264a:** *In Vivo* Characterization of Glucose Responsive Insulin Delivery Systems — **Lisa R. Volpatti**, Morgan Matraga, Abel B. Cortinas, Robert Langer, Daniel G. Anderson**8:18 Paper 264b:** Silica Nanoparticles Enable Oral Delivery of Insulin — **Nicholas G. Lamson**, Adrian Berger, Kathryn A. Whitehead**8:36 Paper 264c:** Targeted, Systemic Dendrimer-Drug Therapies for Age Related Macular Degeneration — Siva Pramodh Kambhampati, Imran Bhuto, Gerard Luttj, **Rangaramanujam Kannan****8:54 Paper 264d:** Growth Rate Dissipation of Metastatic Triple Negative Breast Cancer Attributed to Slow Tumor-Clearing and Deep Tumor-Penetrating Chemotherapy — **Alaina Howe**, Sally Stras, Aprameya Prasad, Stavroula Sofou**9:12 Paper 264e:** Neutrophil-Particle Interactions in Blood Circulation Drive Particle Clearance and Alter Neutrophil Responses in Acute Inflammation — **William Kelley**, Catherine A. Fromen, Margaret Fish, Reheman Adili, Jeffrey Noble, Mark Hoenerhoff, Michael Holinstat, Omolola Eniola-Adefeso**9:30 Paper 264f:** Synthesis and Characterization of pH-Responsive Hydrogels for Oral Delivery of High Isoelectric Point Therapeutic Proteins — **Heidi F. Oldenkamp**, Michael C. Koetting, Nicholas A. Peppas**9:48 Paper 264g:** Zwitterionic Polymer Coatings to Limit Protein Adsorption to Nanocarrier Surfaces — **Jennifer Fiegel**, Benjamin King**10:06 Paper 264h:** High-Throughput Synthesis and Characterization of Rapidly Eroding Polyanhydride Nanoparticle Libraries for Drug Delivery — **Adam Mullis**, Sean Kelly, Sarah Jacobson, Akash Mitra, Balaji Narasimhan**(265) Biosensors, Biodiagnosis and Bioprocess Monitoring: Cell and Protein Detection****Tuesday, Oct 30, 8:00 AM**

Westin Convention Center, Cambria

Adam Melvin, Chair  
Kevin J. Cash, Co-Chair**Sponsored by:** Bioengineering**8:00 Paper 265a:** Integrated Biosensor for Rapid and Point-of-Care Sepsis Diagnosis — **Jouha Min**, Filip Swirski, Hakho Lee, Ralph Weissleder**8:18 Paper 265b:** Development of a Fast-Responding, Minimal-Equipment Biosensor for Zinc Deficiency — **Monica McNeerney**, **Mark P. Styczynski****8:36 Paper 265c:** Non-Invasive Cell Density Measurement of Mammalian Cell Cultures in Early Stage Seed Trains — **Jana McGuin**, Sarah Magnino, Mark Berge, Michael Mollet**8:54 Paper 265d:** Protein Detection with Peptoid-Functionalized Carbon Nanotube Optical Sensors — **Linda Chio**, Jackson Travis Del Bonis-O'Donnell, Mark A. Kline, Ronald N. Zuckermann, Markita Landry**9:12 Paper 265e:** High-Throughput Single Cell Analysis of Deubiquitinating Enzyme Activity in Intact Cells — **Manibarathi Vaitthiyathan**, Nora Safa, Shayan Sombolestani, Adam Melvin**9:30 Paper 265f:** A Handheld Optical Detection Method for Detection of *Vibrio Cholerae* in Environmental Water Samples — **Katherine N. Clayton**, Julia G. Fraseur, Dong Hoon Lee, Taylor Moehling, Steven T. Wereley, Jacqueline C. Linnes, **Tamara L. Kinzer-Ursem****9:48 Paper 265g:** Phenome to Genome Enabled By Microfluidics and High-Throughput Quantitative Microscopy — **Hang Lu****(266) Chemical Modifications and Processing of Biomaterials****Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 325

Yulin Deng, Chair  
Zhaohui Tong, Co-Chair**Sponsored by:** Forest and Plant Bioproducts Division**8:00 Paper 266a:** Cellulose Nanocrystal: Synthesis, Characterization, Dispersion in Organic Media and Surface Modification — **Mohammad J. Hasan**, Ashley Johnson, Esteban E. Ureña-Benavides**8:21 Paper 266b:** Liquid-Liquid Lignin-Solvent Systems: Phase Behavior, Characterization and Applications — **Junhuan Ding**, Spencer Temples, Sallye Gathmann, Mark C. Thies**8:42 Paper 266c:** Preparation of pH-Responsive Latex Films from Glycerol Based Dendritic Precursors for Food Packaging — **Karyn Moses**, Hanxi Bao, William Pelletier, Melanie Correll, Zhaohui Tong**9:03 Paper 266d:** Hydrothermal Carbonization of Biomass: Examination of Post Synthesis Treatment and Characterization Techniques — **Avery Brown**, Michael T. Timko, Geoffrey Tompsett**9:24 Paper 266e:** Development of Bioplasticizers from Soybean Oil — **Lucas Stolp**, Dharm Kodali**(267) Circulating Fluidized Beds and Measurement Techniques****Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 415

Allan Issangya, Chair  
Michael J. Molnar, Co-Chair**Sponsored by:** Fluidization and Fluid-Particle Systems**8:00 Paper 267a:** *Intrusive Probes in Riser Applications* — Ray Cocco, Reddy Karri, T. M. Knowlton, John Findlay, Thierry Gauthier, Christine Hrenya, **Jia Wei Chew****8:18 Paper 267b:** Non-Intrusive Measurement and Imaging of Circulating Fluidized Beds Using Electrical Capacitance Volume Tomography — **Cody Park**, Yaswanth Pottimurthy, Tien-Lin Hsieh, Benjamin Straiton, Mingyuan Xu, Dawei Wang, Qussai Marshdeh, Liang-Shih Fan, Andrew Tong**8:36 Paper 267c:** Method of Estimating the Solids Mass Flow Rate in a Gas-Solids Riser Using the Integrated Mixture Momentum Equation and the Dynamic Pressure Gradient Distribution — **John Paccione****8:54 Paper 267d:** Influence Parameters and Modeling of Solids Circulation Rate in the High-Density Circulating Fluidized Beds — **Xin Su**, Chengxiu Wang, Xingying Lan, Jinsen Gao**9:12 Paper 267e:** Full-Loop Simulation of Gas-Solids Flow in Circulating Fluidized Beds with Different Sizes — **Min Wang**, Yingya Wu, Xiaogang Shi, Xingying Lan, Jinsen Gao**9:30 Paper 267f:** A Very, Very Small-Scale Experiment of Fluidized Particle Segregation: A Prerequisite for the Uncertainty Quantification of CFD-DEM Simulations — **Casey Q. LaMarche**, Steven R. Dahl, William Fullmer, Christine M. Hrenya**9:48 Paper 267g:** Modeling the Hydrodynamics of Tapered Gas-Solid Risers — **Xinhua Liu**, Meng Zhao, Shanwei Hu, Wei Ge**10:06 Paper 267h:** Validation Study on an Eulerian-Lagrangian Method in a Circulating Fluidized Bed — **Yuki Mori**, Mikio Sakai**(268) Colloidal and Soft Matter Hydrodynamics****Tuesday, Oct 30, 8:00 AM**

Omni William Penn Hotel, Frick

Roseanna N. Zia, Chair  
Lilian Hsiao, Co-Chair**Sponsored by:** Fluid Mechanics**8:00 Paper 268a:** Controlling Shear Thickening in Colloidal Dispersions By the Addition of Shaped, Non-Colloidal Particles — **Norman J. Wagner****8:15 Break****8:30 Paper 268d:** Dynamics and Rheology of Suspensions of Particles with Arbitrary Shapes — **Mingyang Tan**, Travis W. Walker**8:45 Paper 268c:** Jamming and Shear Jamming in the Dense Geometrically Rough Suspensions — **Arman Boromand**, Joao Maia, Mark D. Shattuck, Corey S. O'Hern**9:00 Paper 268e:** Permeability in Fractal Colloidal Networks — **Lev D. Gelb**, Alan L. Graham**9:15 Paper 268f:** Enhanced Mass Transfer in Colloidal Systems Is Due to Diffusiophoresis — **P. Sunthar**, Rakhi Dhuriya**9:30 Paper 268g:** Equilibrium and Non-Equilibrium Dissipative Particle Dynamics Simulations of Pluronic/Water Mixtures — **Hermes Droghetti**, Ignacio Pagonabarraga Mora, Paola Carbone, **Daniele Marchisio****9:45 Paper 268h:** Viscoelastic Properties of Polymer Networks from Probe Rheology Simulations: Effect of Network Mesh Size — **Rafikul Islam**, Nestor Valadez-Perez, Tsutomu Indei, Jay D. Schieber, Rajesh Khare

**10:00 Paper 268i:** The Role of End-Plate Wetting in the Filament Formation and Break-up of High Surface Tension, Strain Hardening Fluids — *Ravi Neelakantan, Jerome Unidad, Elif Karatay, Eric Cocker, Ramesh Palghat, David Johnson*

**10:15 Paper 268j:** Dynamics, Rheology, and Breakup of Droplets with Complex Interfaces – Role of Interfacial Viscosity and Bending Resistance — *Vivek Narsimhan*

#### (269) Computational Catalysis I: Fundamentals

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 402

Michail Stamatakis, Chair  
Srinivas Rangarajan, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 269a:** Modelling of the Dynamic Behavior of Catalyst Materials in Reacting Conditions: An Application to the Catalytic Partial Oxidation of Methane on Rhodium — *Raffaele Cheula, Aloysius Soon, Matteo Maestri*

**8:18 Paper 269b:** Effects of Dopant Loading and CO Adsorption on the Structural Stability of Highly Dilute Alloys — *Konstantinos Papanikolaou, Matthew Darby, Michail Stamatakis*

**8:36 Paper 269c:** Unravelling Hydrogenation Barriers for CO<sub>2</sub> Reduction on Nitrogen Doped Zigzag Edges of Graphene — *Yasemin Basdogan, John A. Keith*

**8:54 Paper 269d:** Overcoming Ammonia Synthesis Scaling Relations with Plasma-Enabled Catalysis — *Prateek Mehta, Patrick Barboun, Francisco Herrera, David Go, Jason C. Hicks, William F. Schneider*

**9:12 Paper 269e:** How Do DFT+U and Hybrids Alter Widely Applied Linear Scaling Relations in Heterogeneous Catalysis? — *Qing Zhao, Heather J. Kulik*

**9:30 Paper 269f:** Grand Canonical DFT Investigation of CO<sub>2</sub> Electrorreduction on Noble and Transition Metal Surfaces — *Dominic Alfonso, De Nyago Tafen, Douglas R. Kauffman*

**9:48 Paper 269g:** Determination of H<sub>2</sub>O-Solvated Cationic Fe(III) Coordination Geometry in Fe-SSZ-13 Using Wavefunction Coupled-Cluster Parameterized Hybrid Density Functional Theory — *Sichi Li, William F. Schneider*

**10:06 Paper 269h:** Coverage Dependent Adsorption of Phenol on Pt (111): Estimating the Lateral Interactions Exhibited By Bio-Oil Model Compounds Under Hydrodeoxygenation Reaction Conditions — *Neeru Chaudhary, Alyssa Hensley, Yong Wang, Jean-Sabin McEwen*

#### (270) Continuous Crystallization Processes

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 302

Christopher L. Burcham, Chair  
Xiaochuan Yang, Co-Chair

**Sponsored by:** Crystallization and Evaporation

**8:00** Introductory Remarks

**8:05 Paper 270a:** Development of an Automated Multi-Stage Continuous Reactive Crystallization System with In-Line Pats for High Viscosity Process — *Chuntian Hu, Salvatore Mascia*

**8:28 Paper 270b:** Disturbance Studies of Continuous Cooling Crystallization of Carbamazepine — *Xiaochuan Yang, David A. Acevedo, Adil Mohammad, Naresh Pavurala, Wei-Lee Wu, Eleazar Wong, Thomas O'Connor, Celia N. Cruz*

**8:51 Paper 270c:** Interface Nucleation in Segmented Continuous Crystallization Process — *Yanyan Gao, Ying Wang, Min Su*

**9:14 Paper 270d:** Model Based Process Design on Continuous Cooling Crystallization — *Claire Yiqing Liu, David A. Acevedo, Xiaochuan Yang, Adil Mohammad, Naresh Pavurala, Zoltan K. Nagy, Celia N. Cruz, Thomas O'Connor*

**9:37 Paper 270e:** High Throughput Continuous Crystallization of Lysozyme in an Oscillatory Flow Baffled Crystallizer with Real Time Process Monitoring — *Joseph Oliva, Zoltan K. Nagy*

**10:00 Paper 270f:** Dynamic Modeling of a Continuous Reactive Crystallization Process — *Nima Yazdanpanah, Thomas O'Connor, Celia N. Cruz*

**10:23** Concluding Remarks

#### (271) Conversion of Solid Wastes to Energy and/or Product

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 319

Zheng Liu, Chair  
Hsi-Wu Wong, Co-Chair  
Sudhagar Mani, Co-Chair  
Michael Tai, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**8:00 Paper 271a:** Synthesis of Graphene from Mango Biomass Via PECVD — *Javishk Shah, Maria Carreon*

**8:15 Paper 271b:** Hydrothermal Carbonization of Wet Biomass Materials for the Production of Hydrochar — *Jeremy Taylor, Ross Lee, Matthew Wood, Dan Spracklin, Justinus A. Satrio*

**8:30 Paper 271c:** A Feasibility Study on Biofuel Production Using Anaerobic Digestion and Thermochemical Catalysis — *Ahmad Naqi, John N. Kuhn, Babu Joseph*

**8:45 Paper 271d:** Identifying Co-Products from Guar and Guayule Processing Residues — *Catherine E. Brewer*

**9:00 Paper 271e:** Continuous Calcination of Pyrolysis Oil Derived Renewable Coke in a Rotary Tube Furnace — *Yaseen Elkasabi, Yetunde Sorunmu, Akwasi A. Boateng*

**9:15 Paper 271f:** Experimental Investigation and Process Design for the Conversion of Carbon Black Waste into Valuable Resources — *Zhiyi Yao, He Li, Shin Nuo Koh, Chi-Hwa Wang*

**9:30 Paper 271g:** Thermodynamics and Kinetics for KOH Leaching of Potassium Alunite from Copper tailings — *Meng-Jie Luo, You-Fa Jiang, Ping Li, Xingfu Song, Jianguo Yu*

**9:45 Paper 271h:** Residual Biomass As Feedstock for Production of Fuel or Value Added Products Via Pyrolysis — *Andres Casoni, Victoria Gutierrez, Maria Alicia Volpe, Patricia M. Hoch*

**10:00 Paper 271i:** Manufacture of Sustainable Light-Weight Concrete Blocks By Utilizing Industrial Solid Waste — *Arunima Shukla, Ashok N. Bhaskarwar*

**10:15 Paper 271j:** Aerated Concrete Blocks Production Using Secondary Steelmaking Slag — *Nahla Alamoodi, Lourdes F. Vega, Safiya Khalil, Hamda A. Alblooshi, Alya J. Alzaabi, Meera S. Alqemzi, Mohamed Shahtout, Subramanyam Shivaswamy*

#### (272) Data Mining and Machine Learning in Molecular Sciences I

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 308

Andrew Ferguson, Chair  
Johannes Hachmann, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**8:00 Paper 272a:** Nonlinear Manifold Learning of Nucleosome Dynamics from Molecular Simulation — *Ashley Guo, Joshua Lequieu, Juan de Pablo*

**8:15 Paper 272b:** Machine Learning Predicts Functional Classes of Family 7 Glycoside Hydrolases with High Accuracy — *Japheth Gado, Anna Borisova, Jerry Ståhlberg, Christina M. Payne*

**8:30 Paper 272c:** Implementation and Automation of a Hierarchical Graph Based Approach for Extracting Coarse-Grain Mapping Operators — *Maghesree Chakraborty, Andrew White*

**8:45 Paper 272d:** Machine Learning Algorithms for High-Throughput Chemical Sensing Using Liquid-Crystals — *Yankai Cao, Huaizhe Yu, Nicholas L. Abbott, Victor M. Zavala*

**9:00 Paper 272e:** Materials Informatics for Process Optimization: Case Studies Using P3HT and PP Composites — *Michael McBride, Nils Persson, Elsa Reichmanis, Martha A. Grover*

**9:15 Paper 272f:** Learning Many-Body Molecular Interactions from Machine Learning — *Francesco Paesani, Thuong Nguyen, Andreas W. Götz*

**9:30 Paper 272g:** Combining Machine Learning and Evolutionary Computing for Accelerating Materials Design — *Tarak Patra, David S. Simmons, Subramanian Sankaranarayanan, Badri Narayanan*

**9:45 Paper 272h:** Predicting Colloidal Crystals from Shapes Via Inverse Design and Machine Learning — *Yina Geng, Greg van Anders, Sharon C. Glotzer*



**10:00 Paper 272i:** Autonomous Crystal Structure Characterization with Neighborhood Graph Analysis — **Wesley F. Reinhart, Athanasios Z. Panagiotopoulos**

**10:15 Paper 272j:** The Physical Analytics Pipeline - a Bayesian Optimization of the Hybrid Organic-Inorganic Perovskite Compositional Space — **Henry C. Herbol, Matthias Poloczek, Paulette Clancy**

**(273) Design and Operations Under Uncertainty I**  
**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 410

Nagore Sabio, Chair  
Matthew D. Stuber, Co-Chair

**Sponsored by:** Systems and Process Design

**8:00 Paper 273a:** A Computational Tool for Applying Optimization Under Uncertainty on Advanced Process Simulators — **Frits Byron Soeppan, John C. Eslick, Miguel A. Zamarripa, Andrew Lee, Benjamin P. Omell, Charles H. Tong, Brenda Ng, Jeremy C. Ou, Pedro Sotorrio, Joshua Boverhof, Michael S. Matuszewski, David C. Miller**

**8:19 Paper 273b:** A Novel Objective Reduction Method: Application to the Comparison of Risk Metrics — **Daniel Vázquez, Ruben Ruiz-Femenia, Jose A. Caballero**

**8:38 Paper 273c:** Stochastic Programming Framework for Electric Power Infrastructure Planning — **Cristiana L. Lara, Benjamin P. Omell, David C. Miller, Ignacio E. Grossmann**

**8:57 Paper 273d:** Strategic Planning of Supply Chains Considering Extreme Events: Novel Heuristic and Application to the Petrochemical Industry — **Michael Ehrenstein, Gonzalo Guillén-Gosálbez**

**9:16 Paper 273e:** Resilient Design and Operations of Chemical Process Systems Using Robust Optimization — **Jian Gong, Fengqi You**

**9:35 Paper 273f:** A Mixed-Integer Conic Programming Formulation for Computing the Flexibility Index Under Multivariate Gaussian Random Variables — **Victor M. Zavala, Joshua Pulsipher**

**9:54 Paper 273g:** Modeling for Reliability Optimization of System Design and Maintenance Based on Markov Chain Theory — **Yixin Ye, Ignacio E. Grossmann, Jose M. Pinto, Sivaraman Ramaswamy**

**10:13 Paper 273h:** Novel Method for the Integration of Flexibility and Stability in Design of Chemical Processes Under Parametric Uncertainties — **Ying Chen, Zhihong Yuan, Bingzhen Chen**

**(274) Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems**

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 321

David C. Miller, Chair  
Miguel Zamarripa, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**8:00 Paper 274a:** Efficient Selection of Conventional and Phase-Change CO<sub>2</sub> Capture Solvents Based on Nominal and Off-Design Process Operation — **Theodoros Zarogiannis, Athanasios I. Papadopoulos, Ioannis Tsvintzelis, Panos Seferlis**

**8:21 Paper 274b:** Modular CO<sub>2</sub> Capture from Distributed Oilfield Engines — **Joseph Moate, Tony Neumayer, Phil DiPietro, Charles Womble**

**8:42 Paper 274c:** Application of Dynamic Reduced-Order Modeling and Advanced Process Control on UKY-CAER CO<sub>2</sub> Capture Pilot Plant Using CCSI Tools — **Priyadarshi Mahapatra, Jinliang Ma, Benjamin P. Omell, Michael S. Matuszewski, Jonathan V. Pelgen, Kunlei Liu**

**9:03 Paper 274d:** An Optimization-Based Methodology for the Reduction of Gas Flaring in Shale Oil Production — **Andrés Joaquín Calderon Vergara, Natalie J. Pekney**

**9:24 Paper 274e:** Techno-Economic System Analysis for SOFC/GT Hybrid System Accounting for Degradation Effects — **Haoxiang Lai, Thomas A. Adams II**

**9:45 Paper 274f:** Coal Drying, Mercury Removal, and Stabilization Using Heat from a Nuscale Small Modular Reactor — **Ying Wang, William C. Schaffers, David A. Bell, Jong Suk Kim, Richard Boardman**

**10:06 Paper 274g:** Optimal Design of Gas-Fired Moving-Bed Chemical Looping Combustion Systems — **Anca Ostace, Chinedu O. Okoli, Andrew Lee, Anthony P. Burgard, Debansu Bhattacharyya, David C. Miller**

**(275) Developments in Extractive Separations: Solvents**

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 303

George S. Goff, Chair  
Matthaeus Siebenhofer, Co-Chair

**Sponsored by:** Extractions

**8:00 Paper 275a:** Separation of Volatile Organic Acids from Fermentation Using Non-Ionic Surfactants — **Emmanuel Revellame, Remil Aguda, Samanta Bonilla, Shayla LeBoeuf, Sukanta Mondal**

**8:22 Paper 275b:** Integrated Solvent Design for the Separation of Aromatics from Aliphatics with Ionic Liquids — **Yuanyuan Lyu, Joan F. Brennecke, Mark Stadtherr**

**8:44 Paper 275c:** Separation of Aromatic & Aliphatic Hydrocarbons Using 1-Butyl-3-Methylimidazolium Tricyanomethanide Ionic Liquid — **Ismaila Shittu, Muhammad Khan, Mamoun Althuluth, Maaik C. Kroon, Cornelis Peters**

**9:06 Paper 275d:** A Study on Thermodynamic Properties of Binary Mixtures of Sesame OIL with Aliquat 336 and Tributyl Phosphate — **Soumi Sarkar, Prabirkumar Saha**

**9:28 Paper 275e:** Recovery of Lithium Ion from Salt-Lake Brines Via Solvent Extraction with [Emim][Fsi] As Coextractant — **Yong Wang, Haotian Liu, Jiahui Fan, Zhiyong Zhou, Zhongqi Ren**

**9:50 Paper 275f:** Enhanced Oil-Solid Separation By Multifunctional Switchable Solvents — **Lin He, Ziqi Yang, Xingang Li, Hong Sui, Lin Xu**

**10:12 Paper 275g:** Liquid-Liquid Extraction and Theoretical Binding Studies of Crown Ether Derivatives with Mixed Heteroatoms Towards Platinum Group Metals — **Rey Eliseo C. Torrejos, Rosemarie Ann I. Cuevas, Grace M. Nisola, Min Sang Hoon, Jeong Woo Han, Seong-Poong Lee, Wook-Jin Chung, Teklebrahan G. K. Weldemhret**

**(276) Directed and Self Assembly of Colloids**

**Tuesday, Oct 30, 8:00 AM**  
Omni William Penn Hotel, Conference Center B

Bhuvnesh Bharti, Chair  
Peter J. Belmont, Co-Chair

**Sponsored by:** Interfacial Phenomena

**8:00 Paper 276a:** Buckling Instabilities in Self-Assembled Microsphere-Elastomer Composite Films — **Peng Jiang**

**8:15 Paper 276b:** Phase Diagrams for Mixtures of Dipolar Rods and Disks — **Ryan Maloney, Carol Hall**

**8:30 Paper 276c:** Pressure-Tunable Photonic Band Gaps in an Entropic Colloidal Crystal — **Rose Cersonsky, Julia Dshemuchadse, James Antonaglia, Greg van Anders, Sharon C. Glotzer**

**8:45 Paper 276d:** Self-Assembly By Deionization, Coacervation, and Epitaxy — **Rodrigo Guerra, Paul M. Chaikin**

**9:00 Paper 276e:** Assembly of Paramagnetic Colloids Under Rotating Magnetic Fields: From Their Dynamic to Quasi-Equilibrium Morphologies — **Elaa Hilou, Sibani Lisa Biswal**

**9:15 Paper 276f:** Orientational (Dis) Order in Crystals of Hard Polyhedra — **Julia Dshemuchadse, Andrew S. Karas, Greg van Anders, Sharon C. Glotzer**

**9:30 Paper 276g:** Strain Fields in Repulsive Colloidal Crystals — **Bryan Vansaders, Julia Dshemuchadse, Sharon C. Glotzer**

**9:45 Paper 276h:** Displacive Transformations in Floppy Colloidal Crystals: Unearthing the Role of Hydrodynamic Interactions — **Young Ki Lee, Yifan Wang, John C. Crocker, Talid Sinno**

**10:00 Paper 276i:** Emergence of Traveling Waves in Linear Arrays of Electromechanical Actuators — **Shashank Pandey, Yong Dou, Charles A. Cartier, Kyle J. M. Bishop**

**10:15 Paper 276j:** Identity Crises in Hard Polyhedral Glass-Formers — **Erin G. Teich, Greg van Anders, Sharon C. Glotzer**

**(277) Distillation Processes Fundamentals, Developments, and Applications I**

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 301

Daniel R. Summers, Chair  
Andrew W. Sioley, Co-Chair

**Sponsored by:** Distillation and Absorption

**8:00 Paper 277a:** Minimum Reflux Behavior of Multicomponent Mixture Separation Using Complex Distillation Columns — **Zheyu Jiang, Mohit Tawarmalani, Rakesh Agrawal**

**8:25 Paper 277b:** Control of Non-Key Compositional Bulges in Industrial Distillation Unit Operations — **Isuru A. Udugama, Michael A. Taube, Krist V. Gernaey**



**8:50 Paper 277c:** Synthesis of Distillation-Based Separation Networks Using Block Superstructure — **Jianping Li**, Salih E. Demirel, M. M. Faruque Hasan

**9:15 Paper 277d:** Optimization of Heat-Integrated Multicomponent Distillation Sequences — **Tony Joseph Mathew**, Radhakrishna Tumbalam Gooty, Mohit Tawarmalani, Rakesh Agrawal

**9:40 Paper 277e:** Rigorous Modeling of Chlorine Drying Using Sulfuric Acid — **Quincy Amen**, Paul M. Mathias

**10:05 Paper 185j:** Molecular Tracking: An Alternative Computer-Aided Concept for Multi-Component Distillation Column Design — **Nima Nazemzadeh**, Isuru A. Udugama, Jens Abildskov, Seyed Soheil Mansouri

**(278) Education Division Award Winners: Service, Innovation, and Research (Invited Talks)**  
**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 411

Polly R. Piergiovanni, Chair  
Matthew Liberatore, Co-Chair

**Sponsored by:** Education

**8:00** Introductory Remarks

**8:05 Paper 278a:** A Call to Service — Areas of Focus Where You Can Contribute and Make a Difference to Engineering — **Donald P. Visco Jr.**

**8:35 Paper 278b:** Off-Road Professing: Creating Positive Change in Curriculum and Department Culture from Outside the Tenure Track — **Anthony Butterfield**

**9:05 Paper 278c:** Enthalpy, Entropy, Confused Students & Overworked Faculty-What We've Learned about Students' Misconceptions in Thermal Sciences & Faculty Adoption of Effective Practices — **Margot A.-S. Vigeant**, Michael J. Prince, Kathryn Nottis, Milo D. Koretsky

**9:35** Panel Discussion

**(279) Electroactive Biomaterials to Sense and Control Microbial Infections**  
**Tuesday, Oct 30, 8:00 AM**  
Westin Convention Center, Pennsylvania East

Haluk Beyenal, Chair  
Mark Ehrensberger, Co-Chair

**Sponsored by:** Microbes at Biomedical Interfaces

**8:00 Paper 279a:** Control of Pseudomonas Aeruginosa Biofilms By Electrical Currents Using a Simple Agar Model — **Devendra Dusane**, Varun Lochab, Travis Jones, Casey Peters, Amitava Das, Sashwati Roy, Chandan Sen, Vish Subramaniam, Daniel Wozniak, Shaurya Prakash, Paul Stoodley

**8:18 Paper 279b:** Prevention of Select Escape Pathogens from Attaching to Titanium Using Cathodic Voltage Controlled Electrical Stimulation Combined with Antibiotic Therapy — **Mary Canty**, Nicole Luke-Marshall, Anthony Campagnari, Mark Ehrensberger

**8:36 Paper 279c:** Computational Modeling of Cathodic Voltage Controlled Electrochemical Treatment of Biofilms in-Vivo — **Amir Mokhtare**, Mark Ehrensberger, Edward P. Furlani

**8:54 Paper 279d:** Electroactive Surfaces and Their Use for Biofilm Removal to Advance Wound Healing — **Abdelrhman Mohamed**, Hannah M. Zmuda, Mia Mae Kiamco, Ahmed Ben Sahil, Yash Raval, Douglas R. Call, Robin Patel, Haluk Beyenal

**9:12 Paper 279e:** Toward to the Design of an Electrochemical Therapy (ECT) Against Microbial Infection — **Nna-Emeka Onukwugha**, Eloise Parry-Nweye, Tagbo H.R. Niepa

**9:30 Paper 279f:** Wireless Electrostimulation to Eradicate Bacteria Biofilm — **Hao Wang**, Dacheng Ren

**9:48 Paper 279g:** Electrochemical Detection of Bacterial Biofilms on Titanium — **Caelen Clark**, Mark Ehrensberger

**10:06 Paper 279h:** Novel Focused Multivector Ultraviolet (FMUV) Disinfection without Manual Cleaning and Chemical Disinfection in-between Surgeries and throughout the Hospital Environment — **Donna Armellino**, Luis F. Romo, Thomas J. Walsh, Vidmantas Petraitis, Audrey McNicholas, Wladyslaw Kowalski, Mao-wen Weng

**(280) Electrocatalysis and Photoelectrocatalysis IV: Advances in Fuel Cell Catalysts**  
**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 401

Gang Wu, Chair  
Jason Goodpaster, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 280a:** Stability of Platinum in the Electrochemical Environment: Reconstruction, Roughening, and the Third Peak — **Ian T. McCrum**, Michael A. Hickner, Michael J. Janik, Marc T.M. Koper

**8:20 Paper 280b:** Sustainable Synthesis of Electrocatalytic Bismuth-Based Core-Shell and De-Alloyed Nanoparticles — **Anastasios Angelopoulos**, Kevin Tonniss, Junchuan Fang

**8:40 Paper 280c:** Atomically Dispersed and Nitrogen Coordinated Metal Site Catalysts for Oxygen Reduction in Acids — **Gang Wu**

**9:00 Paper 280d:** Oxygen Reduction Reaction over a Novel 3D Pt-Supported Vertically Aligned Carbon Nanofiber — **Jiayi Xu**, Ayyappan Elangovan, Jun Li, Bin Liu

**9:20 Paper 280e:** PdCu Alloy Nanoparticles As Highly Active Electrocatalysts for Hydrogen Oxidation in Alkaline Electrolyte — **Yang Qiu**, Le Xin, Yawei Li, Ian T. McCrum, Michael Janik, Wenzhen Li

**9:40 Paper 280f:** Recent Developments in Electrochemical Synthesis of Hydrogen Peroxide — **Samira Siahrostami**

**(281) Emerging Technologies in Pharmaceutical Research and Manufacturing**  
**Tuesday, Oct 30, 8:00 AM**  
Westin Convention Center, Washington

Shujauddin M. Changi, Chair  
David A. Acevedo, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**8:00 Paper 281a:** Convergent Synthesis of Peptides at Large Scale — **Nil Tandogan**, Kevin Seibert, Neil Kallman, Jennifer M. Groh, Shankararam Vaidyaraman, Michael Kopach

**8:25 Paper 281b:** Continuous N-Hydroxyphthalimide Mediated Electrochemical Aerobic Oxidation of Benzylic C-H Bonds — **Yiming Mo**, Klavs F. Jensen

**8:50 Paper 281c:** Future Manufacturing Platforms — **Carla Luciani**, Kevin Seibert, Colm O'Mahony, Adam D. McFarland, Krizia Karry, Wyatt Roth, Michael Frederick, Martin Johnson, Sarah O'Keefe, Paul Collins

**9:15 Paper 281d:** Harnessing Power of Membranes to Enable Process Intensification and Improvement — **Manish S. Kelkar**, Daniel Weyant, Rajarathnam E Reddy, John Belletini, Nandkishor K. Nere

**9:40 Paper 281e:** Nanofiltration: Integration in Small and Medium Molecule Processes — **Shujauddin M. Changi**, Nicholas Klitzing, Kevin Seibert, Nil Tandogan, Neil Kallman, Michael Kopach, Carla Luciani, Christopher Lippelt, Justin Burt, Michael Laurila, Josep Martinelli

**10:05 Paper 281f:** Liquid Phase Oligonucleotide Synthesis with Membrane Separation for Efficient Large Scale Manufacturing — **Danilo Cuccato**, Jack H. J. Cordrey, Piers Gaffney, Patrizia Marchetti, Jeong F. Kim, Daniela Negru, Mike Anson, Andrew G. Livingston

**(282) Engineering the Tissue and Cell Microenvironment I: Development and Disease**  
**Tuesday, Oct 30, 8:00 AM**  
Westin Convention Center, Butler

Shreyas Rao, Chair  
Tadas Kasputis, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**8:00 Paper 282a:** Polymer Implant Establishes Novel Microenvironments within Adipose Tissue That Correlate with Enhanced Glucose Metabolism and Protection from Diet Induced Obesity — **Michael Hendley**, Prakasam Annamalai, Michael Gower

**8:18 Paper 282b:** A Miniaturized Organoid Model of Early Liver Development — **Ogechi Ogoke**, Cortney Ott, Allison Kalinousky, Tala Mon, William Pratt, Natesh Parashurama

**8:36 Paper 282c:** Engineering Co-Culture of Cultured Glioblastoma Cells and Astrocytes to Study Cell-Cell Communication in GBM — **Kimberly M Stanke**, Christina Wilson, Erin Eickman, Oleh Khalimonchuk, Srivatsan Kidambi

**8:54 Paper 282d:** Assembly of Human Stem Cell-Derived Vascular Spheroids and Cortical Spheroids to Model 3-D Brain-like Tissues — **Liqing Song**, Xuegang Yuan, Teng Ma, Yan Li

**9:12 Paper 282e:** Radiation-Induced Changes in Normal Tissues Alter Tumor Cell Recruitment — **Benjamin C. Hacker**, Steven M. Alves, Edward E. Graves, Marjan Rafat

**9:30 Paper 282f:** Recapitulating the Effects of Ethanol on an Inflamed Gut-Liver Axis *in Vitro* — **Anjaney Kothari, Padmavathy Rajagopalan**

**9:48 Paper 282g:** Invited Speaker: Engineered Microenvironments to Study Breast Cancer Progression — **Shilpa Sant**

**(283) Environmental Applications of Nanotechnology and Nanomaterials**  
**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 309

Larry Erickson, Chair  
Ryan Hansen, Co-Chair

**Sponsored by:** Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

**8:00 Paper 283a:** Shape Matters: Cr(VI) Removal Using Iron Nanoparticle Impregnated 1-D Vs 2-D Carbon Nanohybrids Prepared By Ultrasonic Spray Pyrolysis — **Nirupam Aich, Arvid Masud, Yanbin Cui, John D. Atkinson**

**8:21 Paper 283b:** Carbon Nanotube-TiO<sub>2</sub> Composites for Photocatalytic Oxidation of Volatile Organic Compounds — **Brian Everhart**

**8:42 Paper 283c:** Synthesis and Characterization of Analyte-Responsive Nanoparticles for the Detection of Polychlorinated Biphenyls — **Dustin Savage, James Z. Hilt, Thomas Dziubla**

**9:03 Paper 283d:** Eco-Friendly Fabrication and Characterization of Mechanically Strong, Thermally Stable, Largely Impermeable and Biodegradable Zein-Graphene Oxide Nanocomposites — **Tahrima B. Rouf, Jozef Kokini**

**9:24 Paper 283e:** Gold on Fractal Nanoparticles As Highly Active Surface-Enhanced Raman Scattering Substrates — **Akram Abbasi, Arijit Bose, Geoffrey D. Bothun**

**9:45 Paper 283g:** Synthesis and Characterization of Cobalt Doped TiO<sub>2</sub>-PVA Nanofibers Catalytic Membrane for Photo Degradation of Congo Red from Aqueous Solution — **Adolph A. Muleja, Bhekile B. Mamba**

**10:06 Paper 283h:** Aerosol Synthesis of Oxygen-Deficient Titania in a Hot-Wall Reactor — **Maximilian Domaschke, Lukas Wergen, Wolfgang Peukert**

**(284) Excellence in Graduate Polymer Research (Invited Talks)**

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 327

Muzhou Wang, Chair  
Megan Robertson, Co-Chair

**Sponsored by:** Polymers

**8:00 Paper 284a:** Photoswitching Polymer Network Topology — **Yuwei Gu, Jeremiah Johnson**

**8:15 Paper 284b:** Dynamics of Polymer-Grafted Nanoparticles Under Soft Confinement — **Ryan Poling-Skutvik, Ali Slim, Suresh Narayanan, Jacinta C. Conrad, Ramanan Krishnamoorti**

**8:30 Paper 284c:** Investigation of Solvent Composition and Salt Addition in High Transference Number Nonaqueous Polyelectrolyte Solutions — **Kyle M. Diederichsen, Bryan D. McCloskey**

**8:45 Paper 284d:** Cononsolvency of the Elastin-like Polypeptide in Binary Aqueous Solutions and Its Application to Protein Purification Processes — **Carolyn Mills, Erika Ding, Bradley D. Olsen**

**9:00 Paper 284e:** Direct Observation of Linear and Circular Polymers in Non-Equilibrium Flows: Single Molecule Studies of Topology and Entanglements — **Yuecheng Peter Zhou, Charles M. Schroeder**

**9:15 Paper 284f:** Understanding Film-to-Wire Transition of Conjugated Polymers Driven By Meniscus Instability — **Ge Qu, Ying Diao**

**9:30 Paper 284g:** Understanding the Interplay between Polymer Architecture and Solvent Quality through Coarse-Grained Molecular Dynamics Simulation and Liquid State Theory — **Thomas Gartner III, Arthi Jayaraman**

**9:45 Paper 284h:** Engineering Polymer-Nanoparticle Systems Towards Sustainable Devices and Sensors — **Bailey Risteen, Justin O. Zoppe, Mohan Srinivasarao, Paul Russo, Elsa Reichmanis**

**10:00 Paper 284i:** Production of Surface-Active Polymer Janus Colloids Via Flash Nanoprecipitation — **Victoria E. Lee, Robert K. Prud'homme, Rodney D. Priestley**

**10:15 Paper 284j:** *S. Oneidensis* As a Living Electrode for Controlled Radical Polymerization — **Gang Fan, Christopher M. Dundas, Austin J. Graham, Nathaniel A. Lynd, Benjamin K. Keitz**

**(285) Fundamentals of Interfacial Phenomena I**

**Tuesday, Oct 30, 8:00 AM**

Omni William Penn Hotel, Conference Center A

Gerold A. Willing, Chair  
Clint P. Aichele, Co-Chair

**Sponsored by:** Interfacial Phenomena

**8:00 Paper 285a:** Synergistic Impact of Polymer/Surfactant Complexation on the Colloidal Depletion Force — **Bhagyashree Lele, Robert D. Tilton**

**8:16 Paper 285b:** Determination of the Interaction Mechanism of 10 Um Oil-in-Water Emulsion Droplets Using Optical Tweezers — **An Chen**

**8:32 Paper 285c:** Friction of Ionic Liquid-Glycol Ether Mixtures at Titanium Interfaces: Negative Load Dependence — **Rong An, Liangliang Huang, Faiz Ullah Shah**

**8:48 Paper 285d:** Contact Electrification: The Phenomenon of Charging at Interfaces — **Siowling Soh**

**9:04 Paper 285e:** A Simple Model for the Wall Depletion Length of Confined DNA — **Aditya Bikram Bhandari, Jeffrey G. Reifengerger, Hui-Min Chuang, Han Cao, Kevin D. Dorfman**

**9:20 Paper 285f:** Microstructural Characterization of Pickering Emulsions Stabilized By Polymer Brush Nanoparticles Via Small-Angle Neutron Scattering — **John K. Riley, Robert D. Tilton, Paul Butler**

**9:36 Paper 285g:** Impact of Humidity on Silica Nanoparticle Agglomerate Morphology and Size Distribution — **Georgios A. Kelesidis, Florian M. Furrer, Karsten Wegner, Sotiris E. Pratsinis**

**9:52 Paper 285h:** Effect of Surfactant Structure on Self-Assembly and Charging Processes in Anhydrous Nonpolar Liquids. — **Keyi Xu, Jae Gang Oh, Paul J. Sides, James W. Schneider, Dennis C. Prieve**

**10:08 Paper 285i:** Role of Molecular Linker in the Self-Assembly of Alkyl Ethoxylate Surfactants — **Andrew M. Bodratti, Junce Cheng, Matthew R. Chow, Stephanie M. Kong, Marina Tsianou, Paschalis Alexandridis**

**(286) Graphene and Carbon Nanotubes: Absorption, Separations, and Transport Processes**

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 310

Geyou Ao, Chair  
Ardemis A. Boghossian, Co-Chair

**Sponsored by:** Carbon Nanomaterials

**8:00 Paper 286a:** Learning How to Predict SWCNT-Recognition DNA Sequences — **Yoon Yang, Ming Zheng, Anand Jagota**

**8:25 Paper 286b:** Characterization of Double-Stranded DNA (dsDNA) on Single-Walled Carbon Nanotubes (SWCNTs) — **Shang-Jung Wu, Nils Schuergers, Kun-Han Lin, Alice Gillen, Clemence Corminboeuf, Ardemis A. Boghossian**

**8:50 Break**

**9:15 Paper 286d:** CNT-Based Carbon Monoxide Sensors with Voltage-Modulated Sensitivity — **Suchol Savagatrup, Vera Schroeder, Timothy M. Swager**

**9:40 Paper 286e:** Self-Assembly of 3D Graphene/Carbon Nanotube Electrodes Via Electrostatic Polyanion Coordination for Biosensor Applications — **Enoch Nagelli, An Vu, Kamil Woronowicz, F. John Burpo, Alexander Mitropoulos**

**10:05 Paper 286f:** Fe<sub>3</sub>O<sub>4</sub>/graphene nanocomposites with Upsurge Superhydrophobic Properties — **Sudheer Yadav, Mu Qiu Wu, Rong An, Tao Feng**

**(287) Industrial Internet of Things (IIoT) Applications and Industry 4.0 Forum**

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 333

Tim Olsen, Chair  
Nima Yazdanpanah, Co-Chair  
Zhenyu Wang, Co-Chair

**Sponsored by:** Next-Gen Manufacturing

**8:00 Welcoming Remarks**

**8:05 Paper 287a:** Industrial Internet of Things (IIoT) Applications and Industry 4.0 (Doug Child, Siemens) — **Douglas Child**

**8:13 Paper 287b:** Industrial Internet of Things (IIoT) Applications and Industry 4.0 (Leo Chiang, Dow) — **Leo H. Chiang**

**8:21 Paper 287c:** Industrial Internet of Things (IIoT) Applications and Industry 4.0 (Richard Braatz, MIT) — **Richard D. Braatz**

**8:29 Paper 287d:** Industrial Internet of Things (IIoT) Applications and Industry 4.0 (Jason Blackburn, Emerson) — **Jason Blackburn**

**8:37 Paper 287e:** Panel Discussion (Tim Olsen, Emerson) — **Tim Olsen**

**(288) In Honor of Neal Chung II: Liquid Separation**

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 304

Yan Wang, Chair  
Yoram Cohen, Co-Chair  
Chuyang Y. Tang, Co-Chair

**Sponsored by:** Membrane-Based Separations

**8:00 Paper 288a:** Intelligent RO Systems: Advances and Challenges — **Yoram Cohen**

**8:21 Paper 288b:** Membrane Materials for Liquid-Based Separations in Water and Organic Solvents — **Suzana P. Nunes**

**8:42 Paper 288c:** A New Insight into the Formation and Impact of Roughness Features in Polyamide Reverse Osmosis Membranes — **Chuyang Y. Tang**

**9:03 Paper 288d:** High-Performance Ceramic Supported Thin Film Composite Membrane for Organic Solvent Nanofiltration — **Lingling Xia, Marcus Weyd, Jeffrey McCutcheon**

**9:24 Paper 288e:** Novel Polyimide Membranes and Their Modification for Pervaporation Applications — **Yan Wang, Sheng Xu**

**9:45 Paper 288f:** Alignment and Immobilization of Functionalized Aquaporins on Polybenzimidazole Nanofiltration Membranes — **Priyesh Wagh, Yinan Wei, Isabel Escobar**

**10:06 Paper 288g:** Surface Functionalization and Peeling-Off Manipulation Generating Diversified Janus Membranes Toward Multifunctional Applications — **Lu Shao, Xiaobin Yang**

**(289) In Honor of Professor D. Ramkrishna's Contributions to Biopharmaceutical Industry (Invited Talks)**  
**Tuesday, Oct 30, 8:00 AM**  
Westin Convention Center, Somerset

Kushal Sinha, Chair  
Nandkishor Nere, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**8:00** Opening Remarks

**8:10 Paper 289a:** Mammalian Cell Culture Broth Clarification and Affinity Capture of Secreted Antibodies in a Novel Single Integrated Process Using a Compact Settler — **Dhinakar Kompala**

**8:30 Paper 289b:** Examples of Model Informed Drug Development in Drug Design and Delivery — **Ramprasad Ramakrishna, Andrew Stein**

**8:50 Paper 289c:** Drug Loading into and Drug Release from pH- and Temperature-Responsive Hydrogels — **Satish Parulekar, Pravin Ninawe**

**9:10** Break

**9:20 Paper 289d:** Modelling Simultaneous Saccharification and Fermentation of Natural Polymers: Population Balance Interlinked with Cybernetic Modelling — **Pankaj Doshi, Yong Kuen Ho, Hak Koon Yeoh**

**9:40 Paper 289e:** An Analytical Solution to the Breakage Problem — **Ragavendra Hari, Meenesh R. Singh**

**10:00 Paper 289f:** Making Tangible Impact through Mathematical Modeling in Bio-Pharmaceutical Industry — **Nandkishor K. Nere, Kushal Sinha, Natarajan Ramasubramanyan**

**10:20** Concluding Remarks by Professor D. Ramkrishna

**(290) Innovation from Beginning to End: Generating Ideas, Working with People, and Managing Projects**  
**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 331

Eldon Larsen, Chair

**Sponsored by:** Management Division

**8:00 Paper 290a:** Innovation from Beginning to End: Generating Ideas, Working with People and Managing Projects — **Eldon Larsen**

**10:00 Paper 108b:** Using Scrum & Cross-Functional Teams to Deliver Disruptive Results — **Austin S. Lin**

**(291) Jumpstart Your Teaching!: Small Teaching Ideas for Course Improvement**  
**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 406

Daniel Anastasio, Chair  
Amanda Simson, Co-Chair

**Sponsored by:** Professional Development Committee Liaison

**8:00 Paper 291a:** Act Now! Operators Are Standing By: Student Pitch Videos — **Margot A.-S. Vigeant**

**8:18 Paper 291b:** By Students for Students: Using Course Projects to Create Learning Materials for Future Classes — **Lucas J. Landherr**

**8:36 Paper 291c:** Using Peer Review to Improve Student Learning Outcomes Associated with Ill-Structured Problems — **Monica H. Lamm**

**8:54 Paper 291d:** Integrating Open-Ended Research Problems into the Classroom Using POGIL-Guided Projects — **Ryan Hansen**

**9:12 Paper 291e:** Increasing Student Interaction with Anonymous Polling — **Kristine Horvat**

**9:30 Paper 291f:** Get in Pairs and Roll the Dice! — **Joan G. Lynam**

**9:48** Panel Discussion

**(292) Materials Chemistry for Biosensors**  
**Tuesday, Oct 30, 8:00 AM**  
Westin Convention Center, Pennsylvania West

B. Reeja Jayan, Chair  
Markita Landry, Co-Chair

**Sponsored by:** Sensors

**8:00 Paper 292a:** Boronate Ester-Based Dynamic Nucleic Acids for Templated Analyte Detection — **Heidi R. Culver, Kelly Kepler, Christopher N. Bowman**

**8:18** Break

**8:36 Paper 292c:** Mechanistic Optimization of Floating Gate Transistors for Biosensing Applications — **Mathew Thomas, Kevin D. Dorfman, C. Daniel Frisbie**

**8:54 Paper 292d:** Computational Optimization of Metal-Organic Framework (MOF) Arrays for Chemical Sensing — **Jenna Gustafson, Christopher E. Wilmer**

**9:12 Paper 292e:** Morpholino Materials for Diagnostic Applications — **Sade Ruffin, Eshan Treasurer, Isabella Hung, Rastislav Levicky**

**9:30 Paper 292f:** Cardiac Troponin I Detection Using Antibody-Immobilized Disposable Cover Glass and AlGaIn/GaN High Electron Mobility Transistors — **Jiancheng Yang, Patrick Carey IV, Fan Ren, Yu-lin Wang, Michael L. Good, Soohwang Jang, Michael A. Mastro, Stephen J Pearton**

**9:48** Break

**10:06 Paper 292h:** Nanostructured Polymeric Membranes for in-Situ Measurement of Exhaled Formaldehyde and Acetone Kinetics As Early-Stage Non-Invasive Markers of Lung Disease — **Anastasios Angelopoulos, Ulzii Badmaarag**

**(293) MOFs, COFs, and Porous Polymer Materials: Synthesis**  
**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 329

Dongxia Liu, Chair  
Satish Nune, Co-Chair

**Sponsored by:** Inorganic Materials

**8:00 Paper 293a:** Controlled Demolition and Reconstruction of Zeolitic Imidazolate Frameworks Via Solvent Assisted Crystal Redemption (SACRed) — **Krishna Chandran Jayachandrababu, Souryadeep Bhattacharyya, David S. Sholl, Sankar Nair**

**8:18 Paper 293b:** Controlling Metal Organic Framework Thin Film Crystallization Using Dynamic Processes — **Gaurav Giri**

**8:36 Paper 293c:** Electrophoretic Nuclei Assembly for Crystallization of High Performance Membranes on Unmodified Supports — **Guangwei He, Kumar Varoon Agrawal**

**8:54 Paper 293d:** Epitaxial Growth of MOF Nanoparticles with Different Metal Centers — **Xinyang Yin, Xueyi Zhang**

**9:12 Paper 293e:** Time Dependent Structural Evolution of Porous Organic Cage CC3 — **Jolie Lucero, Sameh Elsaidi, Ryther Anderson, Ting Wu, Diego Gomez Gualdron, Moises Carreon, Praveen K. Thallapally**

**9:30 Paper 293f:** Control over the Gas Separation Range of Zeolitic Imidazolate Framework-8 Based Membranes: Metal Replacement and Linkage Exchange — **Panagiotis Krokidas, Marcelo Castier, Hae-Kwon Jeong, Ioannis G. Economou**



**9:48 Paper 293g:** Growth of 2-D Porphyrin-Based Metal–Organic Frameworks on Nonwoven Textiles As Effective Adsorbents for Toxic Industrial Chemicals and Chemical Warfare Agent Simulants — **Dennis T. Lee**, *Jovenal Jamir, Gregory W. Peterson, Gregory N. Parsons*

**10:06 Paper 293h:** Design, Synthesis, and Characterization of Functionalized MOFs for Chemical Warfare Agent Capture — **Jonathan Ruffley**, *Isabella Goodenough, Minh Nguyen Vo, Tianyi Luo, Melissandre Richard, Nathaniel L. Rosi, Eric Borguet, J. Karl Johnson*

#### (294) Nanomaterials for Energy Storage I

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 412

Ling Fei, Chair  
Yong Lak Joo, Co-Chair

**Sponsored by:** Nanomaterials for Applications in Energy and Biology

**8:00 Paper 294a:** Computational Electrochemistry of DNA: Effect of Lithium — **Seung Soon Jang**

**8:30 Paper 294b:** Facile and Scalable Fabrication of Sulfur Cathodes Via Air-Controlled Electrospray — **Jin Hong Lee**, *Mounica Jyothi Divvela, Yong Lak Joo*

**8:50 Paper 294c:** Direct Conversion of CO<sub>2</sub> to Carbon Materials for Energy Conversion and Storage — **Yeeun Kim**, *Won Yeong Choi, Jae W. Lee*

**9:10 Paper 294d:** Mn<sub>3</sub>O<sub>4</sub> Nanoarray and Solid Electrolyte Interface Encapsulated Nanoarray Electrodes for High Performance Lithium Sulfur Battery — **Junling Guo**, *Xiaolong Zhang, Xinyu Du, Fengxiang Zhang*

**9:30 Paper 294e:** Gyroidal 3-D Electrochemical Energy Storage Nanoarchitecture — **Jörg G. Werner**, *Gabriel Rodríguez-Calero, Héctor D. Abruña, Ulrich Wiesner*

**9:50 Paper 294f:** Modeling Mechanisms of Nickel Oxide Lithiation Using First Principles Calculations and Classical Nucleation Theory — **Robert Warburton**, *Handan Yildirim, Guennadi Evmenenko, Michael Bedzyk, Maria K. Y. Chan, Paul Fenter, Tim Fister, Jeffrey Greeley*

#### (295) New Frontiers of Molecular Thermodynamics (Invited Talks)

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 307

Rajesh Khare, Chair  
Shekar Garde, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**8:00 Paper 295a:** Introductory Remarks: Frontiers of Molecular Thermodynamics — **Shekar Garde**

**8:05 Paper 295b:** Molecular Modeling of Charged Systems: From Electrolytes to Ionic Liquids and Molten Salts — **Edward Maginn**

**8:40 Paper 295c:** Assembling Polymeric Ionic Liquids: A Balance of Interactions Leading to New Properties — **Rachel A. Segalman**

**9:15 Paper 295d:** Molecular Modeling of Polymer Crystallization: Heterogeneous Nucleation — **Gregory C. Rutledge**, *Alexander Bourque*

**9:50 Paper 295e:** Context-Dependent Hydrophobic Interactions in Water — **Nicholas L. Abbott**

**10:25 Paper 295f:** Concluding Remarks: Frontiers of Molecular Thermodynamics — **Rajesh Khare**

#### (296) Novel Nanostructured Catalytic Materials I

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 403

Steven R. Saunders, Chair  
Siris Laursen, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 296a:** Development of a New Generation of Stable, Tunable, and Catalytically Active Nanoparticles Produced By the in-Situ and Ex-Situ Synthesis Methods — **Jingguang G. Chen**, *Alexander Orlov, Qiyan Wu, Jiajie Cen, Claron Ridge, Michael Lindsay, Eric A. Stach, Anatoly I. Frenkel*

**8:20 Paper 296b:** Switchable Surfactants for the Preparation of Monodisperse, Supported Nanoparticles and the Effects of Calcination on Nanoparticle Characteristics — **Kristin Bryant**, *Steven R. Saunders*

**8:40 Paper 296c:** A Commercially-Viable One-Step Synthesis Method to Prepare MWW Zeolite Nanosheets — **Yunwen Zhou**, *Ming-Feng Hsieh, Jeffrey D. Rimer*

**9:00 Paper 296d:** Photocatalytic Inorganic Core Hedgehog Particles — **Douglas G. Montjoy**, *Joong Hwan Bahng, Aydin Eskafi, Harrison Hou, Ruiyu Jiang, Nicholas A. Kotov*

**9:20 Paper 296e:** Slowing the Kinetics of Alumina Sol-Gel Chemistry for Controlled Catalyst Overcoating and Improved Catalyst Stability and Selectivity — **Yuan-Peng Du**, *Florent Héroguel, Jeremy S. Luterbacher*

**9:40 Break**

**10:00 Paper 296h:** One Step, Steady State Catalytic Conversion of Methane to Methanol Using Copper Zeolites: Kinetics and Site Requirements — **Mark Sullivan**, *Kimberly Dinh, Randall J. Meyer, Pedro Serna, Yuriy Román-Leshkov*

#### (297) Numerical Analyses of Mixing Processes in Bioreactors

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 334

Richard K. Grenville, Chair  
Arthur W. Etchells III, Co-Chair

**Sponsored by:** North American Mixing Forum

**8:00 Paper 297a:** Optimizing Productivity of Bioreactors with Multiphase Simulation on GPUs — **Philipp Eibl**, *Christian Witz, Johannes G. Khinast*

**8:30 Paper 297b:** Flow inside Bioreactors: Comparing Predictions from Lattice-Boltzmann to Experimental Data — **Brian DeVincentis**, *John A. Thomas, Kevin Smith*

**9:00 Paper 297c:** CFD Modeling of Oxygen Dissolution in Bioreactors: Mass Transfer and Population Balance Study in Stirred Tanks — **Gustavo Montoya**, *Shailesh Ozarkar, Bo Sun, Vinay Kumar Gupta, Jay Sanyal, Markus Braun*

**9:30 Paper 297d:** Kinetic Study and CFD Modeling of Anaerobic Bioethanol Fermentation — **Elham Ebrahimiagda**, *Ali Abbaspourtamijani*

**10:00 Paper 297e:** Bubble-Scale Modeling of Gasified Reactors — **Christopher Tyler**, *John A. Thomas*

#### (298) Particle Engineering and Design for Product Value Enhancement

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 413

Ecevit Bilgili, Chair  
Ilgaz Akseli, Co-Chair

**Sponsored by:** Particle Production and Characterization

**8:00 Paper 298a:** Carrier Based Dry Powder Inhaler Formulation – a Particle Engineering Perspective — **Joana T. Pinto**, *Sarah Zellnitz, Eva Roblegg, Amrit Paudel*

**8:17 Paper 298b:** Spray-Dried Nanocomposites and Amorphous Solid Dispersions with Identical Formulation for Comparative Assessment of Drug Dissolution Enhancement — **Mahbubur Rahman**, *Alexander Coelho, Sayali Bhujbal, Faustin Arevalo, Ecevit Bilgili*

**8:34 Paper 298c:** Fabrication of Biodegradable Rod-Shaped Drug Carriers with Modified Two-Step Emulsion Solvent Evaporation Technique — **Hanieh Safari**, *Reheman Adili, Michael Holinstat, Omolola Eniola-Adefeso*

**8:51 Paper 298d:** Surface Engineering of Lactose Particles By Atomic Layer Deposition for Modified Release — **Damiano La Zara**, *Di Zhang, Mike J. Quayle, Gunilla Petersson, Staffan Folestad, J. Ruud van Ommen*

**9:08 Paper 298e:** Improving Blend and Tablet Properties of Binary Mixtures Containing Cohesive and Poorly-Compactable APIs Using Surface Engineered MMC Based Fine Excipients — **Liang Chen**, *Xiaoyi Ding, Siqi Fan, Zizhou He, Rajesh Davé*

**9:25 Paper 298f:** Determination of Flow and Compressibility Properties of Pharmaceutical Powders: Effect of Fines and High Drug Loading — **Patrick Cronin**, *Bernardo Castro Dominguez, Barbara Schaller, Kevin Moroney, Denise Croker, Ahmad Albadarin, Gavin Walker*

**9:42 Paper 298g:** Formulation of Microcarriers for Levodopa Delivery Via the Pulmonary System — **Mahasweta Paul**, *Raymond Lau*



Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AICHEvents app.



**9:59 Paper 298h:** Surface Modification to Improve Drug-Excipient Mixing for DPI Formulation — **Neetu Varun, Chinmay Ghoroi**

**10:16 Paper 298i:** Impregnation of Catalysts with Viscous Metal Solutions Using Experiments and DEM Simulations — **M. Silvina Tomassone, Yangyang Shen, Jiao Yang, William G. Borghard**

### (299) Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 404

Eric G. Moschetta, Chair  
Jonathan McMullen, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 299a:** Photochemical Models for Drug Substance Stability — **Jose E. Tabora, Michael Smith, Yichen Tan, Thomas La Cruz, Antonio Ramirez, Federico Lora Gonzalez, Thiago Carvalho**

**8:25 Paper 299b:** A Study of Photon Transport in Gas-Liquid Flow: Scalability of Photooxidations from the Micro- to the Milli-Scale — **Anca Roibu, Rishi Bharadwaj, Morthala, Tom Van Gerven, Simon Kuhn**

**8:50 Paper 299c:** Photoredox Iridium-Nickel Dual Catalyzed Decarboxylative Arylation Cross-Coupling: From Batch to Continuous Flow Via Self-Optimizing Segmented Flow Reactor — **Hsiao-Wu Hsieh, Connor W. Coley, Lorenz M. Baumgartner, Klavs F. Jensen, Richard I. Robinson**

**9:15 Paper 299d:** Studies Toward Scalable Photochemical Reactions in Flow — **Emily Corcoran, Francois Levesque, Jonathan P. McMullen, John R. Naber**

**9:40 Paper 299e:** Improving Reactor Design for Scaling-up Photoredox Reactions in Flow — **Eric G. Moschetta, Kaid Harper, Shailendra Bordawekar, Steven J. Wittenberger**

**10:05 Paper 299f:** Photon Mediated Coupling Reactions Using Copper Nanocatalysts - Molecular Mechanisms on Homo Coupling and Hetero Coupling Activity — **Ravi Teja, Andishaeh Dadgar, Farshid Mohammadparast, Marimuthu Andiappan**

### (300) Refining and Petrochemical Plant Modelling and Operations Improvements I

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 323

Vladimir Mahalec, Chair  
Wenli Du, Co-Chair  
Mark Darby, Co-Chair

**Sponsored by:** Fuels and Petrochemicals Division

**8:00 Paper 300b:** Integration of Crude-Oil Scheduling and Refinery Planning By Lagrangean Decomposition Approach — **Haokun Yang, David E. Bernal, Ignacio E. Grossmann**

**8:25 Paper 300c:** Optimal Production and Maintenance Scheduling in Olefin Plants — **Min Chen, Qiang Xu, Wang Zhenlei**

**8:50 Paper 300d:** Ready-to-Use Operational Machine Learning in the Process Industry — **Aswin N. Venkat**

**9:15 Break**

**9:40 Paper 300f:** Rolling Horizon Model for Gasoline Blend Planning Under Uncertainty in Demands Using an Updated Inventory Level Position Based on Chance Constraint Formulation — **Mahir Jalanko Jr.**

**10:05 Paper 300g:** Novel Steady State Process Modeling Methodology for Pressure Swing Adsorption — **Michael Sees, Toni Kirkes, Taehun Kim, Joseph Scott, Chau-Chyun Chen**

### (301) Solids Handling and Processing in Particulate Systems

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 414

Sarah E. Mena, Chair  
Pavithra Sundararajan, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**8:00 Paper 301a:** Understanding the Pressure Loss in Wyres for Dust Collection and Vacuum Cleaning Systems — **Yi Fan, Karl Jacob**

**8:18 Paper 301b:** Limiting Flow Rate of Fine Powders through Hoppers – Investigation of Methods to Increase the Flow Rates — **Madhusudhan Kodam, Karl Jacob**

**8:36 Paper 301c:** Prediction of Loss-in-Weight Screw Feeder Performance and Quantification of Failure Modes from Attribute Measurements of Pharmaceutical Materials — **Anthony Tantuccio, Kendall Moyer, David Goldfarb, Sara Koynov, Stephen L. Conway, Robert Meyer**

**8:54 Paper 301d:** The Use of Fine Excipients to Improve the Manufacturability of Pharmaceutical Tablets — **Maxx Capece**

**9:12 Paper 301e:** Deduster® : The Leading Dust and Streamer Removal System — **Amit K. Gautam, William F. Sahrhage III, Joseph Lutz**

**9:30 Paper 301f:** Improved Combustible Dust Minimum Ignition Energy (MIE) Test Method and Prediction Using CFD Simulation — **Purvali Chaudhari, Bharatvaaj Ravi, Pranav Bagaria, Chad Mashuga**

### (302) Sustainable Fuel from Renewable Resources

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 320

Hyun-Tae Hwang, Chair  
Gonzalo Guillén-Gosálbez, Co-Chair

**Sponsored by:** Sustainability

**8:00 Paper 302a:** Integration of Algal Wastewater Treatment with Hydrothermal Liquefaction to Increase Process Net Energy Recovery — **Kwonit Mallick, Feng Cheng, Zheng Cui, Umakanta Jena, Nagamany Nirmalakhandan, Catherine E. Brewer**

**8:20 Paper 302b:** Supply Chains Analysis for Sustainable Production of Aviation and Marine Biofuels: A Comparative Study of Feedstocks, Technologies, Regions, and GHG Emissions — **John A. Posada**

**8:40 Paper 302c:** Hydrochar Obtained from Hydrothermal Carbonization from Lipid Extracted Algae and Its Use As Solid Fuel — **Umakanta Jena, S. Kent Hoekman**

**9:00 Paper 302d:** Benthic Polyculture Biomass from Wastewater Algal Turf Scrubbers As a Feedstock for Bioeconomy — **Ashani Samarutunga, Ryan Davis, Sandeep Kumar**

**9:20 Paper 302e:** Investigation of Biochar Liquefaction to Produce Chemicals and Fuels — **Rahul Kundu, Hema Ramsurn**

**9:40 Paper 302f:** Investigation of Microwave Assisted Transesterification Reactor of Waste Cooking Oil — **ASO Hassan, Joseph D. Smith**

### (303) Sustainable Management and Uses of Post-Consumer Materials and Waste

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 315

Gerardo J. Ruiz-Mercado, Chair  
Jason Trembly, Co-Chair

**Sponsored by:** General

**8:00 Break**

**8:25 Paper 303b:** Super Critical Transesterification of Fats and Lipids Extracted from Dissolved Air Flotation Sludge — **Saptarshi Chakraborty, Christopher L. Kitchens**

**8:50 Paper 303c:** Reaction Engineering Routes to Waste Gasification for Sustainable Living Environments — **Mason Lang, Kristen Reyes, Michael Matrona, Eric Lange, Brianne DeMattia, Uchechukwu Obiako, Jorge E. Gatica**

**9:15 Paper 303d:** Process Analysis of Continuous Catalytic Gasification As a Waste to Energy Alternative — **Mason Lang, Kristen Reyes, Michael Matrona, Eric Lange, Brianne DeMattia, Uchechukwu Obiako, Jorge E. Gatica**

**9:40 Break**

**10:05 Paper 303f:** Integra LCA: An Innovative Tool for Health Risk Assessment of Plastic Waste — **Dimosthenis Sarigiannis, Spyros Karakitsios, Antonis Gypakis, Alberto Gotti**

### (304) The Energy-Water Nexus

**Tuesday, Oct 30, 8:00 AM**  
David L. Lawrence Convention Center, 317

Urmila M. Diwekar, Chair  
Shweta Singh, Co-Chair

**Sponsored by:** Sustainable Energy

**8:00 Paper 304a:** Energy-Water Nexus Study for a Mushroom Farming Initiative in Nigeria — **Quinta Nwanosike Warren**

**8:20 Paper 304b:** Sustainable Optimal Strategic Planning for Shale Water Management — **Jose A. Caballero, Alba Carrero-Parreño, Viviani C. Onishi, Juan A. Reyes-Labarta, Raquel Salcedo-Díaz, Ruben Ruiz-Femenia, Ignacio E. Grossmann**

**8:40 Paper 304c:** A Multi-Objective Energy-Water Nexus Planning Model: A Case Study of the Power Systems in Texas Edwards Aquifer — **Cory Allen, Yaling Nie, Styliani Avraamidou, Efstratios N. Pistikopoulos, Xin Xiao**

**9:00 Paper 304d:** Optimal Use of Thermal Membrane Distillation (TMD) for Treatment of Flowback Water — *Kaiyu Cao, Priscille I. Etoughe, Rajib Mukherjee, Debalina Sengupta, Joseph Sangil Kwon, Mahmoud M. El-Halwagi*

**9:20 Paper 304e:** The Energy-Water Nexus of Thermoelectric Power Generation and Its Impacts in the Muskingum River Watershed in Ohio — *Kyuha Lee, Sami Khanal, Bhavik R. Bakshi*

**9:40 Paper 304f:** Systematic Analysis and Optimization of Water-Energy Nexus — *Spyridon D. Tsolas, M. Nazmul Karim, M. M. Faruque Hasan*

**10:00 Paper 304g:** Thermo-Economic Optimization Based Comparison of Membrane Distillation Vs Mechanical Vapor Recompression for Shale Gas Produced Water Treatment — *Elmira Mohammadi Shamlou, Atoosa Mashayekhi, Radisav Vidic, Vikas Khanna*

**10:20 Paper 304h:** Application of Adsorbate Solid Solution Theory to Design Novel Adsorbents for Arsenic Removal Using Computer-Aided Molecular Design — *Rajat Doshi, Arti A. Rajput, Rajib Mukherjee, Suresh Gupta, Urmila M. Diwekar*

### (305) Theory, Modeling, and Simulation of Nuclear Chemical Processes II

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 326

Maximilian B. Gorenssek, Chair  
Patrick J. Pinhero, Co-Chair

**Sponsored by:** Nuclear Engineering Division

**8:00 Paper 305a:** Density Functional Theory Study of the Tritium Formations on the Surfaces of  $\gamma$ -LiAlO<sub>2</sub> — *Ting Jia, Hari Paudel, Zhi Zeng, Yuhua Duan*

**8:25 Paper 305b:** Modeling of Surface Morphological Evolution of Plasma-Facing Tungsten in Fusion Reactors — *Dwaipayan Dasgupta, Robert Kolasinski, Dimitrios Maroudas, Brian D. Wirth*

**8:50 Paper 305c:** Stability and Interactions of Point Defects in Lithium Metal Oxides for the Tritium-Producing Burnable Absorber Rod Applications — *Yueh-Lin Lee, Jamie Holber, Hari Paudel, Dan C. Sorescu, Yuhua Duan*

**9:15 Paper 305d:** Effects of Flux on Helium Bubble Growth in Plasma-Facing Materials — *Karl D. Hammond, Ian V. Naeger, Derek Ruff, Sophie Blondel, Dimitrios Maroudas, Brian D. Wirth*

**9:40 Paper 305e:** The Long-Term Evolution of H/He Irradiated in W By a Multi-Scale Approach — *Zhi Zeng, Yonggang Li*

**10:05 Paper 305f:** Design and Implementation of a Nuclear Solvent Extraction Plant-Level Simulator — *Valmor F. de Almeida, Kevin Lyon, Taha Azzaoui*

### (306) Topical Plenary: Frontiers in Green Process Engineering (Invited Talks)

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 318

Wei Liu, Chair  
Jian Liu, Co-Chair  
Yizu Zhu, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**8:00 Paper 306a:** Recent Research Progress on Water Decomposition with Renewable Energies (Invited speech) — *Anirudh Balram*

**8:25 Paper 306b:** Advanced Molecular Rebar® Process for More Durable Products — *Emily Cole*

**8:50 Paper 306c:** New Membranes for CO<sub>2</sub> Capture and Water Purification (Green Process Engineering Innovation Leadership Award speech) — *W.S. Winston Ho*

**9:35 Paper 306d:** Methanol to Olefins: From Fundamental to Commercialization (Green Process Engineering Innovation Professional Achievement Award speech) — *Zhongmin Liu*

### (307) Turbulent and Reactive Flows

**Tuesday, Oct 30, 8:00 AM**

Omni William Penn Hotel, Phipps  
Li Xi, Chair  
De-Wei Yin, Co-Chair

**Sponsored by:** Fluid Mechanics

**8:00 Paper 307a:** An Overview of the Stress-Blended Eddy Simulation Method in Ansys CFD (Invited Talk) — *Florian R. Menter, D. Christopher Hill*

**8:30 Paper 307b:** Reynolds Stress Closure for Inertial Frames and Rotating Frames — *Charles A. Petty, André Bénard*

**8:45 Paper 307c:** Turbulent Drag Reduction in Plane Couette Flow with Polymer Additives: A Direct Numerical Simulation Study — *Bamin Khomami, Hao Teng, Nansheng Liu, Xiyun Lu*

**9:00 Paper 307d:** Vortex Dynamics for High Levels of Polymer Drag Reduction: Quantitative Analysis Enabled By a New Vortex-Tracking Algorithm — *Lu Zhu, Li Xi*

**9:15 Paper 307e:** The Role of Helicity in Turbulent Transport of Passive Scalars — *Quoc T. Nguyen, Dimitrios V. Papavassiliou*

**9:30 Paper 307f:** Cross-Gradient Scalar Transport in Turbulent Shear Flows — *Emmanuel Hitimana, Katrine M. Jansen, Zhenping Liu, Michael G. Olsen, Rodney O. Fox, James C. Hill*

**9:45 Paper 307g:** Universal Realizable Anisotropic Prestress Closure for Multiphase Turbulent Flows — *Charles A. Petty, André Bénard*

**10:00 Paper 307h:** Thermal-Hydraulics, Transient Turbulence, and Two-Phase Flows in a Pressurized-Water Small Modular Nuclear Reactor — *Vivek M. Rao, Joseph D. Smith*

**10:15 Paper 307i:** *Ember*: An Open-Source, Transient Reacting Flow Solver with Applications in Turbulent Flames and Strained Extinction — *Alan E. Long, Raymond L. Speth, Ahmed F. Ghoniem, William H. Green*

### (308) Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, 306

Fikile Brushett, Chair  
Daniel V. Esposito, Co-Chair  
Thomas F. Fuller, Co-Chair  
John Harb, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

**8:00 Paper 308a:** An Update on Solid Oxide Fuel Cell Research — *Raymond J. Gorte*

**8:35 Paper 308b:** Tutorial on Efficient Electrocatalytic Conversion of CO<sub>2</sub> to Intermediates Such As CO and Ethylene — *Paul J.A. Kenis*

**9:10 Paper 308c:** Ionic Liquids As Novel Electrolytes for Energy and Green Chemistry Applications — *Elizabeth J. Biddinger*

**9:45 Paper 308d:** Electrokinetics in Simple and Complex Fluids — *Lynden A. Archer*

### (309) WIC 20th Anniversary: Celebrating Women in Chemical Engineering I (Invited Talks)

**Tuesday, Oct 30, 8:00 AM**

David L. Lawrence Convention Center, Spirit of Pittsburgh A

Julianne L. Holloway, Chair  
Bihter Padak, Co-Chair  
LaShanda T.J. Korley, Co-Chair

**Sponsored by:** WIC 20th Anniversary: Celebrating Women in Chemical Engineering

**8:00 Session Introduction**

**8:03 Paper 309a:** AIChE Women's Initiative - Our Past, Our Future — *Caroline C. Reynolds*

**8:24 Paper 309b:** A Unique Chemical Engineering Career in the Energy Industry — *Cynthia Murphy-Ortega*

**8:45 Paper 309c:** From Supercritical Fluids to Ionic Liquids — *Joan F. Brennecke*

**9:06 Paper 309d:** How to Grow Your Career While Balancing on One Foot — *Meagan Lewis*

**9:27 Paper 309e:** Stratification in Colloidal Films and Lessons from Soft Materials for Women in STEM — *Surita Bhatia*

**9:48 Paper 309f:** Vapor Deposited Polymers: From Fundamentals to Commercialization — *Karen K. Gleason*

**10:09 Paper 309g:** Assembly Engineering of Complex Colloidal Crystals — *Sharon C. Glotzer*

### (310) MAC/MFF Real Talk: Navigating the Academic Career Path to Tenure (Ticketed Event)

**Tuesday, Oct 30, 11:00 AM**

Westin Convention Center, Crawford West

Omolola Eniola-Adefeso, Chair  
Reginald E. Rogers Jr., Co-Chair

**Sponsored by:** Minority Affairs Committee (MAC)

### (311) What the Heck Happened? Past, Present & Future Disruptions to the Chemical/Fuels Business (Invited Talks)

**Tuesday, Oct 30, 11:00 AM**

David L. Lawrence Convention Center, Spirit of Pittsburgh B

Cliff Kowall, Chair  
J. Karl Johnson, Co-Chair

**Sponsored by:** Miscellaneous

**11:00 Paper 311a:** The Impact of Shale Gas and Oil on the Chemical Industry — *Jeffrey J. Sirola*

**11:20 Paper 311b:** Sustainable Energy and Chemicals: Past, Present, and Future — **Joseph B. Powell**

**11:40 Paper 311c:** Disruptions: What the Future May Hold — **Scott F. Mitchell**

**12:00 Paper 311d:** Geopolitical Factors Influencing the Evolution of the Chemical Industry — **David West**

**12:20 Paper 311e:** Agility & Resilience: How to Maintain Career Competitiveness in the Changing Chemical Industry — **Antonios Papadourakis**

**12:40** Panel Discussion

**(312) Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture**

**Tuesday, Oct 30, 11:15 AM**  
David L. Lawrence Convention Center, Spirit of Pittsburgh A

Christopher W. Jones, Chair

**Sponsored by:** Awards Committee

**11:15 Paper 312a:** Microscale Engineering of Responsive, Flexible and Reconfigurable Particle Structures — **Orlin D. Velev**

**(313) Advanced Problem Solving in the Chemical Industry IV**  
**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 407

Zdravko Stefanov, Chair

**Sponsored by:** Young Professionals Committee (YPC)

**(314) Advancements in Materials Science for Powder Handling in Pharmaceutical Process Development**

**Monday, Oct 29, 12:30 PM**

Westin Convention Center, Cambria

Mohammad Azad, Chair  
Anil Rane, Co-Chair  
Athanas Koyunov, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**12:30 Paper 314a:** Round Granules of Dimethyl Fumarate By Three-in-One Intensified Process of Reaction, Crystallization, and Spherical Agglomeration in a Common Stirred Tank — **Tu Lee, Chih-Wei Chen**

**12:50 Paper 314b:** Systematic Approach to High Dosage Formulation Development for Continuous Direct Compression — **Barbara Schaller, Kevin Moroney, Bernardo Castro Dominguez, Patrick Cronin, Denise Croker, Gavin Walker**

**1:10 Paper 314c:** Comparing High Drug Loaded Blend and Tablet Property Improvement Via Various Nano-Silica Dry Coating and Excipient Selection — **Kuriakose Kunnath, Zhonghui Huang, Liang Chen, Kai Zheng, Rajesh Davé**

**1:30 Paper 314d:** Evaluation of Segregation Intensity of Pharmaceutical Blends Using Near Infrared Spectroscopy — **Parind Desai, Shreyas Acharya, Kirby Amponsah-Manager**

**1:50** Break

**2:10 Paper 314f:** Powder Flow Analysis Using an Automated Milli-Scale Powder Flow Test — **Trinkle David, Keirnan LaMarche**

**2:30 Paper 314g:** Understanding the Compression Behavior of Blends: The Application of Percolation Threshold Theory and Multivariate Analysis — **Ana L. P. Queiroz, Abina Crean**

**(315) Advances in Computational Methods and Numerical Analysis**  
**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 410

Jinfeng Liu, Chair  
Kamil A. Khan, Co-Chair  
Matthew D. Stuber, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

**12:30 Paper 315a:** Multiscale CFD Model Parallelization with Application to PECVD of Thin Films — **Marquis Crose, Anh Tran, Yangyao Ding, Panagiotis D. Christofides**

**12:49 Paper 315b:** An Analysis of the Nonlinear Behavior of the Autothermal Reactor — **Guilherme Ozorio Cassol Sr., Stevan Dubljevic**

**1:08 Paper 315c:** Accurate and Efficient Discrete Finite Volume Approximations for Population Balances Incorporating Coagulation and Fragmentation — **Mehakpreet Singh, Gurmeet Kaur, Themis Matsoukas, Gavin Walker**

**1:27 Paper 315d:** Comparison of Global, Stochastic Optimization Algorithms Using Toy Problems and Multi-Parameter Models to Kinetic Fermentation and Rheological Data — **Matthew Armstrong, Corey James, April Miller**

**1:46 Paper 315e:** Multilevel Monte Carlo Applied for Efficient Estimation of Observables in Multiscale Stochastic Systems — **Grigoriy Kimaev, Luis A. Ricardez-Sandoval**

**2:05 Paper 315f:** Tightening McCormick Relaxations Via Reformulation of Intermediate Functions into Schema — **Matthew Wilhelm, Robert Ernst, Matthew D. Stuber**

**2:24 Paper 315g:** Optfill: A Novel Optimization-Based Tool to Automate the Gapfilling of Genome-Scale Metabolic Models — **Wheaton Schroeder, Rajib Saha**

**2:43 Paper 315h:** A Novel Homotopy Continuation Technique to Locate All Real Solutions of a Nonlinear System of Algebraic Equations — **Saeed Khaleghi Rahimian, J. D. Seader**

**(316) Advances in Enzymatic Catalysis II**

**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 405

Andrew J Adamczyk, Chair  
Heather Mayes, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 316a:** Single-Molecule Characterization of Czyme Protein Modules Adsorption to Multivalent Glucan Polymers like Cellulose — **Shishir Chundawat, Bhargava Nemmaru, Mark Hilton, Markus Hackl, Cesar Lopez, Gnana Gnanakaran, Matthew Lang**

**12:59 Paper 316b:** Combinatorial Experimental and Computational Approach for the Effective Entrapment of Glucose Oxidase in Hyaluronic Acid Nanogels — **Jordan Chapman, Ahmed E. Ismail, Cerasela Zoica Dinu**

**1:18 Paper 316c:** Spatiotemporal Dynamics from a Classic Enzyme Cascade with Self-Governing Substrate Competition — **Yifei Zhang, Stanislav Tsitkov, Henry Hess**

**1:37 Paper 316d:** Uncovering the Quantum Mechanical Origins of Enzymatic Catalysis with Systematic QM/MM Methods and Accelerated, Large-Scale Electronic Structure — **Heather J. Kulik, Zhongyue Yang, Rimsha Mehmood, Mengyi Wang, Helena Qi**

**1:56 Paper 316e:** Towards Scalable Production of Enantiomerically Pure Amines: Enzyme Mechanism and Kinetics — **Robert D. Franklin, John M. Robbins, Joshua Whitley, Andreas S. Bommarius**

**2:15 Paper 316f:** Construction of Artificial Metalloenzyme Catalyst and the Study of Size Effect — **Xiaoyang Li Jr., Jun Ge**

**2:34 Paper 316g:** Functionalized Magnetic Graphene Oxide Sheets for Efficient Cota Laccase Immobilization — **Chunzhao Liu**

**(317) Advances in Metabolic Engineering: Emerging Tools and Technologies**

**Tuesday, Oct 30, 12:30 PM**

Westin Convention Center, Westmoreland West-Central

Ryan Summers, Chair  
Kevin V. Solomon, Co-Chair  
Mark Blenner, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 317a:** Automated Cellular Engineering of *Saccharomyces Cerevisiae* Strains with High Resistance and Production of Lactic Acid — **Yajie Wang, Tong Si, Huimin Zhao, William Streyer**

**12:48 Paper 317b:** A Comparative Analysis of Single Cell and Droplet-Based FACS for Improving Production Phenotypes: Riboflavin Overproduction in *Yarrowia Lipolytica* — **Legian Liu, James Wagner, Shuo-Fu Yuan, Maya Venkataraman, Adam Abate, Hal Alper**

**1:06 Paper 317c:** Utilization of the Endogenous Toxin Gene for Selection of High Performing Microbial Cells for Bioproduction Enhancement — **Xiaonan Wang, Avaniek Cabales, Zhenghong Li, Haoran Zhang**

**1:24 Paper 317d:** Alleviation of Enzyme Product Inhibition By Genetic Biosensor-Based Evolution and Its Application in Enhanced Cis,Cis-Muconic Acid Production in *Pseudomonas Putida* — **Ramesh Kumar Jha, Niju Narayanan, Scott Patrick Henelly, Naresh Pandey, Christopher Johnson, Gregg T. Beckham, Taraka Dale**

**1:42 Paper 317e:** Cell-Free Prototyping Tools for Rapid Biosynthetic Pathway Engineering — **Ashty S. Karim, Michael Köpke, Michael C. Jewett**

**2:00 Paper 317f:** Syntrophic Co-Culture Amplification of Production Phenotype for High-Throughput Screening of Microbial Strain Libraries — **Tatyana Saleski, Alissa Kerner, Meng Ting Chung, Corine Jackman, Azzaya Khasbaatar, Katsuo Kurabayashi, Xiaoxia (Nina) Lin**

**2:18 Paper 317g:** Regulatory Tools and Strategies to Boost Microbial Production — **Yajun Yan**



**(318) Applications of Molecular Modeling to Study Interfacial Phenomena II****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 308

Vance Jaeger, Chair  
Harold W. Hatch, Co-Chair  
Jindal K. Shah, Co-Chair**Sponsored by:** Computational Molecular Science and Engineering Forum**12:30 Paper 318a:** Development of Interface Potential Based Methods for Calculating the Wetting Properties of Complex Systems — *Karnesh Jain, Andrew J. Schultz, Jeffrey R. Errington***12:45 Paper 318b:** Molecular Dynamics Analysis of Salt Effect on Anti-Agglomerant Surface Adsorption in Natural Gas Hydrates — *Hadi Mehrabian, Michael A. Bellucci, Bernhardt L. Trout***1:00 Paper 318c:** Adsorption and Self-Assembly of Surfactant Molecules on Metallic Surfaces Studied Using Molecular Simulations — *Sumit Sharma, Xueying Ko***1:15 Paper 318d:** Rationalizing Stability and Doping of Atomically Precise Ligand-Protected Metal Nanoclusters — *Michael G. Taylor, Qi Li, Rongchao Jin, Giannis Mpourmpakis***1:30 Paper 318e:** Influence of Chlorine Adsorption on the Thermodynamic Wulff Shape of Ag Nanocrystals — *Kristen Fichthorn, Tonnam Balankura***1:45 Paper 318f:** Computational Studies of Novel Structure-Directing Agents and Crystal Growth Modifiers for Zeolite Catalysts — *R. John Clark, Jeremy C. Palmer***2:00 Paper 318g:** Gas Transport at the Polymer-Zeolite Interface Using Atomistic Simulations — *Ravi C. Dutta, Suresh K. Bhatia***2:15 Paper 318h:** Comparative Analysis of Surface Configurations of CO Adsorbed on hcp and fcc Cobalt for the Fischer-Tropsch Synthesis — *Greg Collinge, Norbert Kruse, Catherine Stampfl, Jean-Sabin McEwen***2:30 Paper 318i:** Atomistic Modeling Strategies for Solid Electrolyte Interphase Formation and Properties in Lithium Ion Batteries — *Mathew J. Boyer, Gyeong S. Hwang***2:45 Paper 318j:** Geometric Surface Tension Probed By Molecular Dynamics Simulation of Lennard-Jones Rods, Spheres, and Dyads Thereof — *Jane J. Ou, Mitchell Anthamatten, Shaw H. Chen***(319) Biocolloids, Biomolecules, and Nanomaterials of Medical Relevance****Tuesday, Oct 30, 12:30 PM**

Westin Convention Center, Pennsylvania East

Nancy J. Lin, Chair  
Jacinta Conrad, Co-Chair**Sponsored by:** Microbes at Biomedical Interfaces**12:30 Paper 319a:** Mechanisms Contributing to the Formation of "Floating Biofilms" in Staphylococcus Aureus Orthopedic Infections (Invited Talk) — *Michael Otto***12:48 Paper 319b:** Bacteria Adhesion Is Mechanosensitive to Polymer Coating Properties (Invited Talk) — *Jessica Schiffman***1:06 Paper 319c:** Invited Talk 3: Prospective Technologies Targeting Microbial Biofilm and Its Microenvironment — *Hyun Koo***1:24 Paper 319d:** Investigating the Interfacial and Metabolic Properties of Bacteria at Hexadecane-Water Interfaces — *Nicholas Waters, Sricharani Balmuri, Tagbo H.R. Niepa***1:42 Paper 319e:** Complex Liquid Emulsions and on-Chip Ring Resonators for Bacteria Detection — *Suchol Savagatrup, Timothy M. Swager***2:00 Paper 319f:** Native Airway Mucus Rheology in Health and Patients with Cystic Fibrosis Having Positive or Negative Microbial Culture — *Matthew R. Markovetz, Marianne Muhlebach, Ian Garbarine, Charles R. Esther, Richard C. Boucher, David B. Hill***2:18 Paper 319g:** Engineering Biology to Make Novel Antimicrobials — *Cesar de la Fuente-Nunez***2:36 Paper 319h:** Association with Outer Membrane Vesicles Drastically Alters Bacterial Toxin Activity — *Angela C. Brown, Elnaz S. Rasti, Justin Nice, Shannon Collins***(320) Biomolecular Engineering****Tuesday, Oct 30, 12:30 PM**

Westin Convention Center, Cambria

Kevin J. Cash, Co-Chair  
Mehmet A. Orman, Co-Chair**Sponsored by:** Engineering Fundamentals in Life Science**12:30 Paper 320a:** Roles of Variable Linker Length in Dual Acting Virucidal Entry Inhibitors on HIV-1 Potency Via on-the-Fly Free Energy Molecular Simulations — *Steven T. Gossert, Bibek Parajuli, Irwin Chaiken, Cameron F. Abrams***12:48 Paper 320b:** Engineering Ligand-Activated Fusogens from Influenza Hemagglutinin — *Mauricio Valverde, Marti Tooley, Eric T. Boder***1:06 Paper 320c:** Site-Specific Immobilization and Orientation Control of scFv-Fc Antibodies for Ultra-Sensitive Detection of Influenza Virus — *Yoichi Kumada, Natsumi Kamiyoshi, Koichi Takahashi, Shinya Ogasawara, Fumio Gondaira, Jun-ichi Horiuchi***1:24 Paper 320d:** Evolution-Guided Design of Phosphatase Inhibitors — *Michael Hjortness, Laura Riccardi, Akarawin Hongdusit, Alex Ruppe, Mengxia Zhao, Edward Y. Kim, Peter H. Zwart, Banumathi Sankaran, Haribabu Arthanari, Marcelo Sousa, Marco De Vivo, Jerome M. Fox***1:42 Paper 320e:** Improving Aptamer Specificity with Stringent Counterselection Methods — *Jonah Rosch, Franklin Gong, Daniel Balikov, Ethan Lippmann***2:00 Paper 320f:** Viable but Non-Culturable and Persistence Describe the Same Bacterial Stress State — *Jun-Seob Kim, Nityananda Chowdhury, Ryota Yamasaki, Thomas Wood***2:18 Paper 320g:** Invited Speaker: Bio-Nanomanufacturing of Protein Therapeutics Using Biomembrane Microfluidics — *Susan Daniel***(321) Biosensor Devices: Applications I****Tuesday, Oct 30, 12:30 PM**

Westin Convention Center, Pennsylvania West

Qingshan Wei, Chair  
Kevin J. Cash, Co-Chair**Sponsored by:** Sensors**12:30 Paper 321a:** Invited Talk: Advancing Biosensing with Hybrid Nanomaterials and Machine Learning — *Alexander Star***1:00 Paper 321b:** Viscosity Measurement at the Point-of-Need: A Smartphone Capillary-Based Approach — *Jose C. Contreras-Naranjo, Vijetha Nagendra Prakash, Xiaorui Dong, Victor M. Ugaz***1:20 Paper 321c:** Corona Phase Molecular Recognition Sensors in Marine Organisms for Physiological Biologging: A Feasibility Study — *Michael A. Lee, Nathan Chan, Freddy T. Nguyen, Naveed Bakh, Kelvin K. Jones, Crystal Pham, Pablo Garcia-Salinas, Daniel Garcia-Parraga, Vicente Marco, Michael Strano***1:40 Paper 321d:** Detection of Beta Carotene and Lutein Using Electrochemical Impedance Spectroscopy — *Sabrina Marnoto, Jeffrey M. Halpern***2:00 Paper 321e:** A New Surface Functionalized Biosensor for Long-Term *In Vivo* Glucose Monitoring — *Yikun Huang, Yi Luo, Haomin Liu, Donghui Song, Qiuchen Dong, Jing Zhao, Yu Lei***2:20 Paper 321f:** Mobile Technology Based ECL Biosensor Instrumentation — *Daniel Marsh, Hyun J. Kwon***2:40 Paper 321g:** Electrochemical Detection of Extracellular Bacterial Compounds Using Capillary Electrophoresis — *Martin K. Kimani, Edgar D. Goluch*



**(322) Breakthroughs in C1 to Chemicals and Processing Engineering****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 318

Zhongmin Liu, Chair  
David A. Bell, Co-Chair  
Emily Cole, Co-Chair**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment**12:30 Paper 322a:** Catalytic Aromatization of Bio-Derived Liquid Under Methane Environment — *Aiguo Wang, Danielle Austin, Hua Song***12:55 Paper 322b:** Wave Liquefaction™ Processing of Carbon Materials for the Production of Value-Added Chemicals and Feedstocks: Spectroscopic Diagnostics and Material Characterization — *Randy Vander Wal, Arupnanda Sengupta, Madhu Singh, Kurt Zeller, George Skoptsov***1:20 Paper 322c:** Hydrocarbon Chain Growth Via a Nonthermal Electrical Plasma Microreactor — *Ian Reddick, Goran Jovanovic, Alexandre Yokochi, Nick AuYeung, Matthew Young Coblyn, Yu Miao, Omar Mohamed, Adam Shareghi, Andrew Traverso, Anthony Pyka***1:45 Paper 322d:** Combined Experimental and Density Functional Theory Studies on the Modified SrTiO<sub>3</sub> Catalysts for Oxidative Coupling of Methane — *Seo Yeon Lim, Jae-Wook Choi, Dong Jin Suh, Kwang Ho Song, Hyung Chul Ham, Jeong-Myeong Ha***2:10 Paper 322e:** Process Technology Assessment for Mega Scale Projects — *Yizu Zhu, Mohammad Shafiei***(323) Carbon Nanofibers and Related Structures from Renewable and/or Cheap Feedstock and Their Applications****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 310

Evan J. Granite, Chair  
Ioannis Zuburtikudis, Co-Chair**Sponsored by:** Carbon Nanomaterials**12:30 Paper 323a:** Coal to Carbon Fiber — *Matthew Weisenberger***12:55 Paper 323b:** Carbon Nanofibers from a Blend of Lignin with Recycled PET: Properties and Characterization — *Efstathios Svinterikos, Mohamed Al Marzouqi, Ioannis Zuburtikudis***1:20 Paper 323c:** Supercritical Fluids As Reaction Media for Scalable Production of Carbon Nanomaterials — *Haider Almkhelfe, Placidus B. Amama***1:45 Paper 323d:** From Carbon Nanotube Liquid Crystalline Solutions to Functional Fibers — *Vida Jamali, Farnaz Niroui, Matteo Pasquali, A. Paul Alivisatos***2:10 Paper 323e:** Metal Organic Frameworks Promise High Activity and Stability of Carbonic Anhydrase in Synthetic Environment — *Qian Liu, Aisheng Huang, Jordan Chapman, Kenneth Chandler Williams, Nagasree Garapati, Cerasela Zoica Dinu***(324) Catalyzing the Unique Abilities of Students with Disabilities (Invited Talks)****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 411

Christopher Pope, Chair  
Anthony Butterfield, Co-Chair  
Lucas J. Landherr, Co-Chair  
Tianxing Cai, Co-Chair**Sponsored by:** Education**12:30 Paper 324a:** Invited Talk No. 1: Title and Abstract to be Announced — *Ted A. Conway***12:55 Paper 324b:** Presentation from the Science & Engineering Leadership Initiative and Research Experience for Undergraduate Chemistry Students at the University of Delaware (Tentative) — *Karl S. Booksh, Sharon Rozovsky***1:20 Paper 324c:** Invited Talk No. 3: Speaker, Title, and Abstract to be Announced —**1:45 Paper 324d:** Practical Adaptations for Teaching Students with Disabilities — *Ashley Neybert***2:10 Paper 324f:** Invited Talk No. 5: Speaker, Title, and Abstract to be Announced —**2:35 Paper 324g:** Invited Talk No. 6: Speaker, Title and Abstract to be Announced —**(325) Colloidal Dispersions****Tuesday, Oct 30, 12:30 PM**

Omni William Penn Hotel, Conference Center B

Ubaldo M. Córdova-Figueroa, Chair  
Yoonjee Park, Co-Chair  
Xue Chen, Co-Chair**Sponsored by:** Interfacial Phenomena**12:30 Paper 325a:** Quantification of Ligand-Shell Structure on Colloidal PbS Quantum Dots — *Samuel W. Winslow, Yun Liu, James Swan, William A. Tisdale***12:45 Paper 325b:** Asphaltene Mesoscale Aggregation Behavior in Organic Solvents: A Brownian Dynamics Study — *Mohammad Ahmadi, Hassan Hassanzadeh, Jalal Abedi***1:00 Paper 325c:** Tunable Assembly of Gold Nanorods in Polymer Solutions to Generate Controlled Nanostructured Materials — *Jacinta C. Conrad, Ryan Poling-Skutvik***1:15 Paper 325d:** Concentrated Dispersion Behavior in Aqueous Particle/Polymer Systems Observed in Microfluidic Devices — *Blake J. Bleier, Lynn M. Walker***1:30 Paper 325e:** Using Close-Packed Vesicular Dispersions (CPVDs) for Stabilizing Suspensions of Dense Particles Against Sedimentation — *An-Hsuan Hsieh, David S. Corti, Elias I. Franses***1:45 Paper 325f:** Universal Scaling of Quench-Dependent Dynamics in Intermediate Concentration Colloidal Gels — *Subramanian Ramakrishnan, Divya Bahadur***2:00 Paper 325g:** Brownian/Ballistic Motion of Charged Colloidal Particles in the Proximity of Charged Surfaces — *Juan Manuel Hernandez Meza, Angeles Ramirez-Saito, Said E. Aranda Espinoza, Rodrigo Velez-Cordero, B. Jose Luis Arauz-Lara, Bernardo Yanez Soto***2:15 Paper 325h:** ZnO Nanoparticle Morphology in the Stability and Properties of O/W Emulsions — *Tomás-Eduardo Chávez-Miyauchi, Adriana Benítez-Rico, Martín Romero-Martínez***2:30 Paper 325i:** Sculpting Diffusiophoretic Migration with Reactive Solutes — *Xiaoyu Tang, Nan Shi, Anirudha Banerjee, Todd M. Squires***(326) Composites for Environmental Applications****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 329

Zhe Wang, Chair  
Tuo Ji, Co-Chair  
Xinxin Zhao, Co-Chair**Sponsored by:** Composites**12:30 Paper 326a:** Hexavalent Chromium Removal from Water Via Composite Nanofibers — *Yang Lu, Seungwoon "Paul" You, Steven Diklich, Zhanhu Guo, Evan K. Wujcik***12:48 Paper 326b:** Novel and Natural Oil Spill Dispersant Based on the Cactus-Mucilage — *Fei Guo, Sylvia Thomas, Ryan Toomey, Norma Alcantar***1:06 Paper 326d:** Effect of Synthesis Condition of Thermoresponsive Polymer/Magnetic Particle Composite on Its Cu(II) Ion Recycling Property — *Junichi Ida, Risako Sakai, Kodai Hayashi, Tatsushi Matsuyama***1:24 Paper 326e:** Novel Gel Material for Atmospheric Water Absorbent — *Shichao Jiao, Joseph J. McCarthy***1:42 Break****1:52 Paper 326f:** Montmorillonite-Modified Aromatic Polyamide Membrane Materials with Chlorine Resistance — *Holly A. Stretz, Abdulmajeed Altalhi***2:10 Paper 326g:** Preparation of Al/Zr Pillared Bentonite/Cordierite Honeycomb Monolith Reactors for Environmental Application — *Siwela Jeffrey Baloyi***2:28 Paper 326h:** Interfacial Surface Energy Study of the PVC/TiO<sub>2</sub>-HNTs Ultrafiltration Membrane for Its Suitability As an Antifouling Membrane — *Mausumi Mukhopadhyay, Gourav Mishra***2:46 Paper 326i:** A Quick-Fix Design of Phase Change Material By Particle Blending and Spherical Agglomeration — *Tu Lee, Chih-Lin Wang, Kuan-Lin Yeh, Chih-Wei Chen, Yun Lee, Hung-Lin Lee*Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.

**(327) Computational Catalysis II: Metal and Alloy Catalysis****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 402

Matthew M. Montemore, Chair  
Heather J. Kulik, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**12:30 Paper 327a:** Pd As an Oxidation State Modifier and Cocatalyst for the Re-Catalyzed Heterogeneous Deoxydehydration — **Andreas Heyden, Yongjie Xi****12:48 Paper 327b:** First-Principles Modeling of Single-Atom Catalysis: CO Oxidation over Atomically Dispersed Pt on CeO<sub>2</sub> — **Yifan Wang, Ya-qiong Su, Jin-Xun Liu, Ivo Filot, Konstantinos Alexopoulos, Dionisios G. Vlachos, Emiel J.M. Hensen****1:06 Paper 327c:** DFT and Microkinetic Comparison of Pt, Pd and Rh(111) for Catalytic Ammonia Oxidation — **Hanyu Ma, William F. Schneider****1:24 Paper 327d:** Face-Centered Tetragonal Pt Alloys of Fe & Co As Potential Catalysts for ORR — **Shubham Sharma, Andrew A. Peterson****1:42 Paper 327e:** Electronic Effects on Open Framework Material-Encapsulated Metal Nanoparticles (NP@OFM) and Implications on Catalysis — **Benjamin Schweitzer, Chloe Archuleta, Diego Gomez Gualdrón****2:00 Paper 327f:** CO<sub>2</sub> Reduction on Ligand-Protected Au Nanoclusters — **Giannis Mpourmpakis, Natalie Austin****2:18 Paper 327g:** Mechanistic Insights into Non-Oxidative Ethane Dehydrogenation on Pt-Based Catalysts Via First-Principles Microkinetic analysis — **Talin Avanesian, Dionisios G. Vlachos****2:36 Paper 327h:** Predictive Model for Catalyst Effect of Photo-Induced and Copper-Catalyzed Atom Transfer Radical Polymerization (ATRP) Reaction — **Cheng Fang****(328) Continuous Processing Technologies Applied in Drug Substance Manufacturing I****Tuesday, Oct 30, 12:30 PM**

Westin Convention Center, Somerset

Marimuthu Andiappan, Chair  
Cuixian Yang, Co-Chair**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum**12:30 Paper 328a:** Multidimensional Dynamic Experiments in Flow As a Kinetic Platform for Data Rich Experimentation in Pharmaceutical Process Development — **Brian M. Wyvratt, Jonathan P. McMullen, Shane T. Grosser****12:52 Paper 328b:** Autonomous Reaction Platform for Continuous Chemical Synthesis — **Dale Thomas, Connor W. Coley, Victor Schultz, Justin Lummiss, Jonathan Jaworski, Luke Rogers, Anastasios J. Hart, Klavs F. Jensen, Timothy Jamison****1:14 Paper 328c:** Advancing Flow Chemistry Portability: Approach to Crossing the Chasm — **John R. Naber, Francois Levesque, Nicholas Rogus, Glenn Spencer, Plamen Grigorov, Jonathan P. McMullen, David A. Thaisrivongs, Ian W. Davies****1:36 Paper 328d:** Development of a Fixed Bed, Gas Liquid Flow Reactor for Pharmaceutical Applications — **Jason Mustakis****1:58 Paper 328e:** Multiscale Modeling of a Plug Flow Reactor for a Continuous Drug Substance Manufacturing Process — **Nima Yazdanpanah, Thomas O'Connor, Celia N. Cruz****2:20 Paper 328f:** Integrated Quality By Design for Continuous Pharmaceutical Manufacturing: Accounting for Dynamics and Feedback — **Lucas Foguth, Eranda Harinath, Joel Paulson, Richard D. Braatz****2:42 Paper 328g:** Material Tracking in a Fully Continuous Drug Substance Process — **Carla Luciani, Stephen B. Jeffery, Jon Dieringer, Robert Manson, Edmond Kennedy, Aoife Corrigan, Martin Johnson, Scott A. May****(329) CO<sub>2</sub> Capture, Utilization, and Disposal: Key to Clean Energy Production****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 324

Jason Morgan, Chair  
Ryan Anderson, Co-Chair**Sponsored by:** Transport and Energy Processes**12:30 Paper 329a:** Keynote Presentation — **Chuck Sisti****12:51 Paper 329b:** Solar Thermochemical CO<sub>2</sub> Splitting Using Ce<sub>2</sub>Zn<sub>1-x</sub>O<sub>2</sub> Derived Via Co-Precipitation Method — **Rahul Bhosale, Gorakshnath Takalkar****1:12 Paper 329c:** Successful Demonstration of Illinois Industrial Carbon Capture and Storage in a Saline Reservoir — **Sai Gollakota, Scott McDonald****1:33 Paper 329d:** Chemical Looping Combustion (CLC)-Aided Biomass Gasification for Co-Production of Hydrogen and Electricity — **Hari C. Mantripragada, Goetz Vesper, Naoko Ellis, C. Jim Lim****1:54 Paper 329e:** Molecular Insights into the Enhanced Rate of CO<sub>2</sub> Absorption to Produce Bicarbonate in Aqueous 2-Amino-2-Methyl-1-Propanol (AMP) — **Haley Stowe, Gyeong S. Hwang****2:15 Paper 329f:** Improved Plant Efficiency and Reduced Process Complexity in a Coal-Fueled 50 Kwth Chemical Looping Combustion System with a Unique Spouted Fluidized Bed Reactor — **Amanda Warriner, Zhen Fan, Liang Kong, Jonathan V. Pelgen, Heather Nikolic, Kunlei Liu****2:36 Paper 329g:** CO<sub>2</sub>-Based e-Fuels - a Comparative TEA of Methanol & Omes Based on a Novel Assessment Guideline — **Arno W. Zimmermann, Emre Gençer, Stavros Michailos, Katy Armstrong, Johannes Wunderlich, Georg A. Buchner, Annika Marxen, Henriette Naims, Prof. Dr. Reinhard Schomäcker, Francis O'Sullivan, Peter Styring****(330) Crystallization of Pharmaceutical and Biological Molecules****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 302

Mo Jiang, Chair  
Li Tan, Co-Chair**Sponsored by:** Crystallization and Evaporation**12:30** Introductory Remarks**12:35 Paper 330a:** Kinetic Study for Comprehensive Understanding of Solid State Phase Transitions of Nicotinamide/Pimelic Acid Co-Crystals — **Yong Joon Lee, Brandon L. Weeks****12:55 Paper 330b:** Case Study: Modifying API Crystal Habit to Improve Flowability — **Daniel A. Green, Jennifer Tansey, Yan Sun****1:15 Paper 330c:** Tailoring Desired Powder Properties in Pharmaceutical Development By Hswm-Facilitated Polymorph Transformation — **Tyler Wilson, Troy Reynolds, Brandon Brown, Bal Kang, Stacy Bremner, Michael Ischay, Chiajen Lai****1:35 Paper 330d:** Solution Coating of Pharmaceutical Nanothin Films and Multilayer Nanocomposites with Controlled Morphology and Polymorphism — **Prapti Kafle, Elizabeth M. Horstman, Paul J.A. Kenis, Ying Diao****1:55 Paper 330e:** Optimization of Cooling Crystallization of an Active Pharmaceutical Ingredient Undergoing Degradation — **Kanjakha Pal, Zoltan K. Nagy****2:15 Paper 330f:** Antisolvent and Cooling Crystallization of Pharmaceuticals Using a Continuous-Flow Microfluidic Platform — **Paria Coliaie, Meenesh R. Singh****2:35 Paper 330g:** A Case of a Twisty Route to First Crystals — **Lotfi Derdour****(331) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 317

Gerardo J. Ruiz-Mercado, Chair  
Fengqi You, Co-Chair  
Debalina Sengupta, Co-Chair**Sponsored by:** Sustainable Energy

**12:30 Paper 331a:** Toward Supply Chain Optimization of Renewable Energy Carriers — **William W. Tso**, C. Doga Demirhan, Haneol Song, Seungyeon Lee, Joseph B. Powell, Efstratios N. Pistikopoulos

**12:52 Paper 331b:** Methods for Quantitative Consideration of Ecosystem Services in Supply Chain Design and Optimization — **Daniel Garcia**, Fengqi You

**1:14 Paper 331c:** Superstructure-Based Optimization of Carbon Dioxide Conversion and Utilization Via Syngas Intermediate — **Manali Zantye**, M. M. Faruque Hasan

**1:36 Paper 331d:** Heuristic Algorithm Utilizing Mixed-Integer Linear Programming to Schedule Electric Vehicles for Reduced Cost and Energy Use — **Andras Eles**, **Heriberto Cabezas**, Istvan Heckl

**1:58 Paper 331e:** Integrated Power Systems Capacity and Transmission Planning with High Spatial and Temporal Resolution — **Clara F. Heuberger**, Praveen Bains, Niall Mac Dowell

**2:20 Paper 331f:** The Potential of Cooperative Game Theory for the Design of Chemical Supply Chain Networks Under the Carbon Trading Scheme — **Raquel Salcedo-Diaz**, Ruben Ruiz-Femenia, Jose A. Caballero

### (332) Distillation Processes Fundamentals, Developments, and Applications II

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 301

Daniel R. Summers, Chair  
Andrew W. Sioley, Co-Chair

**Sponsored by:** Distillation and Absorption

**12:30 Paper 332a:** Experimental Study and Results of Liquid Distribution Profiles in Large Scale Distillation Column with Structured Packing — **Kazutoshi Ishizaki**, Hitoshi Kihara, Nobuaki Egoshi

**12:55 Paper 332b:** Experimental and Simulation Study on Start-up of Dividing Wall Column for High Purity Separation of Alcohols — **Jiangwei Xie**, Chunli Li, Fei Peng, Honghai Wang, Jing Fang

**1:20 Paper 332c:** Optimal Design and Operation of Four-Product Dividing-Wall (Kaibel) Distillation Column — **Abdallah Alshammari**, Farrukh Ilyas Abid

**1:45 Paper 332d:** Dual-Dividing Wall Column R&D and Deployment — **Robert Piszczek**, Michael L. Hergenrother, Sundar Narayanan, Rustom Billimoria

**2:10 Paper 332e:** Modeling of Liquid Distribution in Random Packed Columns — **Florian Hanusch**, Robert Kender, Volker Engel, **Sebastian Rehfeldt**, Harald Klein

**2:35 Paper 332f:** Energy and Economic Analyses of a Vapor Recompression Distillation System for I-Butane/n-Butane Separation — **Kanwal Shabbir**, **Muhammad Faheem**

### (333) Division Plenary: Major Separations Challenges

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 305

Isaac Gamwo, Chair  
George G. Chase, Co-Chair

**Sponsored by:** Separations Division

**12:30 Paper 333a:** Challenges and Opportunities of Nano-Aerosol Filtration Using Nanofiber Filter — **Wallace Woon-Fong Leung**

**1:10 Paper 333b:** The Advancement and Challenges of Solid/Liquid Separation in the Process Industry — **Wu Chen**

**1:50 Paper 333c:** Membrane Technology in Bioprocessing -- Current Applications and Future Opportunities — **Andrew L. Zydney**

**2:30 Paper 333d:** Replacing Phase Changing Separations: Revisiting Ammonia Manufacturing — **Mahdi Malmali**

### (334) Electrocatalysis and Photoelectrocatalysis V: Oxygen Evolution Reaction

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 401

Samira Siahrostami, Chair  
Maureen H. Tang, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 334a:** An Efficient and Novel Earth-Abundant Oxygen-Evolving Electrocatalyst Based on Self-Supported Amorphous Metal Boride — **Jean Marie Vianney Nsanzimana**

**12:50 Paper 334b:** Metal-Modified Transition Metal Nitride Electrocatalysts for Oer, HER, and Other Reactions — **Brian M. Tackett**, Jingguang G. Chen, Qian Zhang

**1:10 Paper 334c:** Combining Electrochemistry and Surface Science to Identify Electrocatalytic Structure-Property Relationships — **Douglas R. Kauffman**, Xingyi Deng, Dominic Alfonso, Junseok Lee, Dan C. Sorescu, Christopher Matranga

**1:30 Paper 334d:** Active Structures and Species of Modified Oxide Catalysts for the Oxygen Evolution Reaction (OER) — **Bruce E. Koel**

**1:50 Paper 334e:** Lowering the Charge Overpotentials in Li-O<sub>2</sub> Battery By Tailoring the Oxygen Reduction and Evolution Reaction Energetics Using Non-Precious Metal Oxide Electrocatalysts — **Samji Samira**, Ayad Nacy, Eranda Nikolla

**2:10 Paper 334f:** Density Functional Theory Study of Oxygen Evolution Reaction on Specific Terminated Facets of Perovskite Oxides — **Nicholas Apodaca**, **Pabitra Choudhury**

**2:30 Paper 334g:** Core-Shell Nanoparticles for Efficient Oxygen Evolution Electrocatalysis in Alkaline and Acidic Media — **Alaina Strickler**, Maria Escudero-Escribano, Thomas F. Jaramillo

### (335) Electrochemical Fundamentals: Faculty Candidate Session

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 306

Maureen H. Tang, Chair  
Yushan Yan, Co-Chair  
Vijay Ramani, Co-Chair  
William E. Mustain, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

**12:30 Paper 335a:** Cryo-Electron Microscopy for Battery Materials — **Yuzhang Li**, Yi Cui

**12:45 Paper 335b:** Aqueous Electrode-Decoupled Redox Flow Battery System Utilizing Earth Abundant Elemental Actives — **Shrihari Sankarasubramanian**, Yunzhu Zhang, Cheng He, Vijay Ramani

**1:00 Paper 335c:** Evaluation of Temperature Effect on Graphite Anodes for K-Ion and Li-Ion Batteries — **Ryan A. Adams**, Arvind Varma, Vilas G. Pol

**1:15 Paper 335d:** First-Principles Modeling of Anode/Electrolyte Interfaces in Beyond Li-Ion Batteries — **Jeffrey S. Lowe**, Donald J. Siegel

**1:30 Paper 335e:** Operando Study of the LiV<sub>2</sub>O<sub>6</sub> Cathode: Coupling Electrochemical and Exrd Measurements with Mathematical Models — **Nicholas W. Brady**, Qing Zhang, Andrea Bruck, David Bock, Christian Alexander Gould, Amy C. Marschilok, Kenneth J. Takeuchi, Esther S. Takeuchi, Alan C. West

**1:45 Paper 335f:** Marcus Type Electron Transfer between Molecular Dopants and Pristine (n,m) Single-Walled Carbon Nanotubes at the Solid-Liquid Interface — **Albert Tianxiang Liu**, Yuichiro Kunai, Anton Cottrill, Volodymyr Koman, Pingwei Liu, Daichi Kozawa, Xun Gong, Michael Strano

**2:00 Paper 335g:** Integrating Energy Storage Systems into Renewable Grids -- a Model Based Approach — **Seong Beom Lee**, Chintan Pathak, Venkatasailanathan Ramadesigan, Wenzhong Gao, Venkat R. Subramanian

**2:15 Paper 335h:** Lithium Ion Solvation and Electrodeposition in Ternary Ionic Liquid Electrolytes for Lithium Metal Batteries — **Qianwen Huang**, Burcu Gurkan

**2:30 Paper 335i:** Ionic Liquids and Dilute Electrolytes: The Surprising Connection — **Matthew A. Gebbie**

**2:45 Paper 335j:** Design of New Electrolytes for Lithium-Sulfur Batteries — **Chibueze Amanchukwu**, Zhenan Bao

### (336) Enabling and Advanced Formulations in Drug Product Processing I: Focus on Dissolution

**Tuesday, Oct 30, 12:30 PM**

Westin Convention Center, Washington

Brendon G. Ricart, Chair  
Kristin J. Ploeger, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**12:30 Paper 336a:** Griseofulvin-Laden Extrudates Prepared Via Nanoextrusion: Impact of Dry-Milling on Dissolution Enhancement — **Ecevit Bilgili**, Meng Li, Casey Furey, Jeffery Skros, Rajesh Davé

**12:51 Paper 336b:** The Effect of Inorganic Salt on Disintegration of Tablets with High Loadings of Kollidon® VA64-Based Amorphous Solid Dispersion — **Hanmi Xi**, Jie Ren, Julie Novak, Eric Kemp, Greg Johnson, Jerry R. Klinzing, Mary Ann Johnson, Wei Xu



**1:12 Paper 336c:** Miniaturized Formulation and Processability Screening for the Rational Design of Ethylene Vinyl Acetate Based Co-Extrudates — **Ioannis Koutsamanis**, Simone Eder, Stefan Mohr, Karin Eggenreich, Michela Beretta, Amrit Paudel, Klaus Nickisch, Maika Friedrich, Eva Roblegg

**1:33 Paper 336d:** Advances in Dissolution Modeling for Oral Dosage Forms with Amorphous Solid Dispersions — **Pedro Valente**, Mafalda Paiva, Ricardo Sousa, João Henriques, Márcio Temtem

**1:54 Paper 336e:** Modeling the Bead-Dissolution Kinetics for Composite Melt-Spray Congealed (MSC) Multiparticulates — **Avik Sarkar**, Brian Shoemaker

**2:15 Paper 336f:** Linking Process, Product and Performance By Raman Imaging Analysis — **Patricia Nunes**, Mafalda Paiva, Pedro Valente, Ana Aguiar-Ricardo, Constança Cacela, Márcio Temtem, **Susana Campos**

**2:36 Paper 336g:** Repurposing Pollen Grains for Oral Delivery of Biologics — **Pedro Gonzalez-Cruz**, Shantanu V. Lale, Md Jasim Uddin, Shashwati Atwe, Noureddine Abidi, Harvinder Singh Gill

**(337) Engineering the Tissue and Cell Microenvironment II: Directing Cell Behavior with Extracellular Cues**  
**Tuesday, Oct 30, 12:30 PM**  
Westin Convention Center, Butler

R. Chase Cornelison, Co-Chair  
Whitney L. Stoppel, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**12:30 Paper 337a:** Vascularization of Pancreatic Islet-Mimetic Organoids with Microvessel Fragments — **Connor Wiegand**, Bo Lin, Joseph E. Candiello, Prashant Kumta, Kaushal Rege, Jay Hoying, Ipsita Banerjee

**12:48 Paper 337b:** Collagen-Elastin Scaffolds for Heart Valve Tissue Engineering — **Xinmei Wang**, Helen Scott, George Mendiola, Mir Ali, **Carla M. R. Lacerda**

**1:06 Paper 337c:** Aligned and Conductive 3D Collagen Scaffolds for Skeletal Muscle Tissue Engineering — **Ivan M. Basurto**, Mark A. Mora, George J. Christ, **Steven R. Caliari**

**1:24 Paper 337d:** Extracellular Forces Tune Actomyosin Contractility to Regulate Fibroblast Migration and Persistence — **Christopher Yankaskas**, Panagiotis Mistriotis, Konstantinos Konstantopoulos

**1:42 Paper 337e:** Geometrically Modulated Substrates Direct Cell Migration and Multicellular Assembly — **Zhu Cheng**, Anand Jagota, Matthew Paszek

**2:00 Paper 337f:** Decoupling Cellular Response to Topography and Stiffness in Three Dimensions — **Colin D. Paul**, Alex Hruska, Jack R. Staunton, Hannah A. Burr, Nancy Jiang, Kandice Tanner, Jiyun Kim

**2:18 Paper 337g:** Invited Speaker: Engineering Glycocalyx to Promote Atheroprotective Endothelium Function — **Eno E. Ebong**

**(338) Environmental Implications of Nanomaterials: Biological Interactions**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 309

Cerasela Zoica Dinu, Chair  
Todd Stueckle, Co-Chair

**Sponsored by:** Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

**12:30 Paper 338a:** A Framework for Assessing the Adequacy of Information for Environmental Impact Assessment of Engineered Nanomaterials — **Muhammad Bilal**, Yoram Cohen, **Michelle Romero-Franco**, Hilary Godwin

**12:49 Paper 338b:** Human Serum Protein Corona Greatly Changes the Interactions between Nanoparticles and a Model Human Erythrocyte (RBC) Membrane — **Nasim Ganji**, Geoffrey D. Bothun

**1:08 Paper 338c:** Membrane Lipid Asymmetry Regulates Nanoparticle-Induced Cell Membrane Damage in Red Blood Cells — **Saeed Nazemidashtarjandi**, **Amir M. Farnoud**

**1:27 Paper 338d:** Assessing Organomodified Nanoclay Pulmonary Toxicity across Its Life Cycle Using Integrated *in Vitro* / *In Vivo* Approaches — **Todd Stueckle**, Alixandra Wagner, Jake Jensen, Eun Gyung Lee, Cerasela Zoica Dinu

**1:46 Paper 338e:** Interactions and Toxicity of Next Generation Graphene-Metal Nanohybrids at the Pulmonary Interfaces: Influence of Emerging Physicochemical Properties — **Nirupam Aich**, Qixin Wang, Arvid Masud, Yun Wu

**2:05 Paper 338f:** Unraveling the Role of Nitrogen in the Biological Activity of Nitrogen-Doped Graphene — **Yan Wang**, Nathalia Aquino de Carvalho, Leanne Gilbertson

**(339) Extractive Separations Fundamentals and Design**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 303

Matthaeus Siebenhofer, Chair  
Megan E. Donaldson, Co-Chair  
George S. Goff, Co-Chair

**Sponsored by:** Extractions

**12:30 Paper 339a:** Hydraulics of Taylor-Couette Disc Contactors — **Annika Grafschafter**, Matthaeus Siebenhofer

**12:55 Paper 339b:** Non-Invasive Analysis of Hydrodynamics and Mass-Transfer in Liquid-Liquid Extraction By Means of Computed Tomography — **Thilo Kögl**, Wolfgang Arlt

**1:20 Paper 339c:** Influence of Surfactants on Mass Transfer and Fluid Dynamics in Disperse Multiphase Systems — **Joschka M. Schulz**, **Matthias Kraume**

**1:45 Paper 339d:** Separation Efficiency and Design Optimization of Gravity Settlers – CFD Modeling and Experimental Investigation — **Evgenia Charlafti**, Jan Steinhoff, David Leleu, Laura Reinecke, Hans-Jörg Bart, Andreas Pfennig, Matthias Kraume

**2:10 Paper 339e:** Liquid-Liquid Equilibrium for Biodiesel-Glycerol-Methanol or Ethanol Systems Using Unifac Correlated Parameters — **Mario Andres Noriega**, **Paulo Cesar Narváez Rincón**, **Alberto Claudio Habert**

**2:35 Paper 339f:** Optimization of the Extraction Parameters in a Millichannel-Based Packed and Unpacked Rectangular Serpentine Extraction Device — **Subrata Kumar Majumder**

**(340) Functional Nanoparticles**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 413

Yangchuan Xing, Chair  
Da Deng, Co-Chair

**Sponsored by:** Nanoparticles

**12:30 Paper 340a:** Estrogen Receptor-Targeted Multiplexing Photoacoustic Polymeric Nanoparticles for Diagnostic and Treatment of Breast Cancer — **Carolina Salvador-Morales**

**12:55 Paper 340b:** Engineering of Charge Transfer Complex Nanocrystals By Electrocrystallization — **Mohamed Kilani**, Korosh Torabi, Guangzhao Mao

**1:20 Paper 340c:** Silica-Coated, Near-UV Activated YVO<sub>4</sub>:Eu<sup>3+</sup>, Bi<sup>3+</sup> Nanophosphors for Dynamic Cell Imaging — **Georgios A. Sotiriou**

**1:45 Paper 340d:** Stimuli Responsive Nano-Agents: From Drug Delivery to Oil and Gas Industry — **Afman Mashat**, Amr Abdel-Fattah, Nan Shi

**(341) Fundamentals and Applications for Hazardous Waste Treatment**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 320

Ramesh Chawla, Chair  
Eunsung Kan, Co-Chair  
Robert W. Peters, Co-Chair

**Sponsored by:** Solid and Hazardous Waste

**12:30 Paper 341a:** Application of Shewanella Biofilms for the Dissimilatory Reduction of Iodate in Groundwater — **Jyothirmai J. Simhadri**, Patrick Ymele-leki

**12:48 Paper 341b:** Cost Effective Removal of Chemically Toxic Dyes Using Micro-Organism from Activated Sludge: Understanding Sorption Mechanism, Kinetics and Associated Thermodynamics — **Arijit Sengupta**, Mohanad Kamaz, Perla Rocha, Xianghong Qian, S. Ranil Wickramasinghe

**1:06 Paper 341c:** Phytoremediation of Cr-Contaminated Soil: Use of Chelators in Cr Phytoextraction — **Sandra Cutts**, Dr. Karolina Mukhtar, Dr. Fanny Coutelot, Dr. John Seaman, Dr. Robin Brigmon, Dr. Robert W. Peters

**1:24 Paper 341d:** Enhancement of Oily Sludge Biodegradation in Historic Refinery Wastewater Lagoons — **Matthew L. Alexander**, Maheswari Chandrasekaran, Najem Alarwan

**1:42 Paper 341e:** Reactive Fe Mineral Coatings in Redox Transition Zones — **Lisa Axe**, Han Hua, Xin Yin, Donna Fennell, Frank Burns

**2:00 Break**

**2:18 Paper 341f:** Exploitation of Alkaline Solid Wastes for CO<sub>2</sub> Mineralization and Utilization: Challenges, Advances and Opportunities — **Shu-Yuan Pan**, Pen-Chi Chiang, Yi-Hung Chen, Kinjal Shah, Tse-Lun Chen

**2:36 Paper 341g:** Enhanced Biosorption of Heavy Metals through Base Treated Coconut Husk — **Ayyaz Ahmad**, M. Ajaz Ahmad, Mahboob Ahmed Aadil, Terán Hilaes Ruly



**Paper 376l:** Thermo-Responsive Ionic Liquids with LCST-Type Phase Transition Property As Draw Solutives in Forward Osmosis for Seawater Desalination — **Hana G. Zeweldi**, Anelyn Bendoy, Lawrence A. Limjuco, Hanseung Kim, Myoung Jun Park, Ko Kyong Shon, Wook-Jin Chung, Grace M. Nisola

**Paper 376m:** Hybrid Zeolitic-Imidazolate Frameworks (ZIFs) Membranes with Tunable Gas Separations — **Febrian Hillman**, Jordan Brito, Hae-Kwon Jeong

**Paper 376n:** A Scalable Method to Prepare Zeolitic-Imidazolate Framework ZIF-8 Membranes on Polymer Hollow Fibers for Propylene/Propane Separation — **Mohamad Rezi Abdul Hamid**, Hae-Kwon Jeong

**Paper 376o:** Membrane Synthesis and Process Design for Hydrogen Purification from Coal-Derived Syngas — **Yang Han**, W.S. Winston Ho

**Paper 376p:** Synthesis and Techno-Economic Analysis of Novel Facilitated Transport Membrane for Post-Combustion Carbon Capture — **Yang Han**, W.S. Winston Ho

**Paper 376q:** Fabrication of Spiral-Wound Membrane Modules for CO<sub>2</sub> Capture from Flue Gas — **Witopo Salim**, Varun Vakharia, Yuanxin Chen, Dongzhu Wu, Yang Han, W.S. Winston Ho

**Paper 376r:** A Combined Seeding Approach for High-Flux Zeolitic-Imidazolate Framework ZIF-67 Membranes for Olefin/Paraffin Separation — **Jingze Sun**, Hae-Kwon Jeong, Kumar Varoon Agrawal, Chen Yu

**Paper 376s:** Microscopic Diffusion of Ethylene in ZIF-11 Based Mixed Matrix Membranes (MMMs) By Pulsed Field Gradient (PFG) NMR — **Evan M. Forman**, Amineh Baniani, Lei Fan, Kirk J. Ziegler, Erkang Zhou, Fengyi Zhang, Ryan Lively, Sergey Vasenkov

**Paper 376t:** Novel High-Performance Hollow Fiber Membrane Modules for Water Desalination through Direct Contact Membrane Distillation — **Mahdi Mohammadi Ghaleni**, Abdullah Al Balushi, Mona Bavarian, Siamak Nejati

**Paper 376u:** Multilayer Composite Membranes with Superior CO<sub>2</sub> Separation Properties — **Ahmad Arabi Shamsabadi**, Hossein Riazi, Saeed Laki, Yuriy Y. Smolin, Yawei Li, Swarnendu Chatterjee, Joshua Snyder, Masoud Soroush

**Paper 376v:** Properties, Processing and Performance of Aromatic Ionic Polyimides and Polyamides As Gas Separation Membranes — **Grayson P. Dennis**, Kathryn E. O'Harra, Jason E. Bara

**Paper 376w:** Rapid Synthesis of Hybrid Zeolitic-Imidazolate Frameworks (ZIFs) Membranes with Tunable Gas Separations — **Febrian Hillman**, Jordan Brito, Hae-Kwon Jeong

**Paper 376x:** Organic Solvent Nanofiltration Via Zeolitic-Imidazolate Framework Membranes: Insights from Molecular Simulation — **Wan Wei**, Krishna M. Gupta, Jianwen Jiang

**Paper 376y:** Separation of Zinc and Nickel from Industrial Wastewater through Supported Liquid Membrane Using Environmentally Benign Solvent — **Supriyo Kumar Mondal**, Manoj Kumar Beriya, Prabirkumar Saha

**Paper 376aa:** A Novel Cationic Guanidine Compound Grafted Polyvinylidene Fluoride Membrane for Biofouling Mitigation — **Shanshan Zhao**, Guimei Liu, Fanggang Meng

**Paper 376ab:** Star Polymers As a New Building Block for the Fabrication of Reverse Osmosis and Nanofiltration Membranes — **Chan Hyung Park**, Sungkwon Jeon, Sang-Hee Park, Sung-Joon Park, Dal-Yong Kim, Jung-Hyun Lee

**Paper 376ac:** Effect of Pressure and Spacer Configuration on Assisted Reverse Osmosis Performance — **Sara Osipi**, Argimiro Resende Secchi, Cristiano P. Borges

**Paper 376ad:** Crystal Morphology and Process Control of Multiple High-Salinity Wastewater Treatment Via Membrane Distillation Crystallization — **Guannan Li**, Gaohong He, Xiaobin Jiang

**Paper 376af:** Membrane-Based Controlled Release: A Useful Tool in Oilfield Operations — **Jimoh K. Adewole**

**Paper 376ag:** Modeling and Optimization of Membrane Based Process for CO<sub>2</sub> Separation from Flue Gas — **Young-Hwan Chu**, Jeong-gu Yeo, Jung-Hyun Lee

**Paper 376ah:** Molecular Simulation Study of Polymers of Intrinsic Microporosity Nanofilms for Organic Solvent Nanofiltration — **Qisong Xu**, Jianwen Jiang

**Paper 376ai:** A Phase Field Method for Mesoscopic Modeling of Porous Polymer Membrane Formation Via Phase Inversion — **M. Rosario Cervellere**, Paul Millett, David Ford, Xianghong Qian, Yuanhui Tang

**Paper 376aj:** Molecular Simulation on Separation of CO<sub>2</sub>/CH<sub>4</sub> Mixture By Carbon Membrane with Zigzag Pore Structure — **Yanqiu Pan**, Liu He, Wei Wang, Tonghua Wang

**Paper 376al:** Combined Concentration Polarization and Pore-Flow Modeling to Predict the Performance of a Nano Filtration Membrane for NaCl Rejection — **Saikat Bhattacharjee**, Sirshendu De

**Paper 376am:** Investigation of Oceanic Microfiber Pollution and Development of Inexpensive Filtration Units to Reduce That from Residential and Commercial Washing Machines — **Ryan Smith**, Ruben Savizky

**Paper 376an:** Electrospun Polyvinylidene Fluoride Membranes for Direct Contact Membrane Distillation — **Sebastian Olarte**, Carson Gattenby, DaJohn Murray, Keith M. Forward

**Paper 376ao:** Modeling the Effects of Mass Transfer on Microstructure Formation in Polymer Membranes — **Douglas Tree**, Lucas Francisco Dos Santos, Glenn H. Fredrickson

**Paper 376ap:** Enhancing Ionic Conductivity of Anion Exchange Membrane Via Incorporating Tetra-Quaternized Calix[4]Arene — **Wanting Chen**, Xuemei Wu, Xiaozhou Wang, Gaohong He

**Paper 376aq:** Highly Hydroxide Conductive Quaternized Polybenzimidazole Anion Exchange Membranes — **Xiaozhou Wang**, Xuemei Wu, Gaohong He, Wanting Chen, Xue Gong, Tiantian Li

**Paper 376ar:** One-Step Formation of Polyethersulfone Inner-Selective Hollow Fiber Membranes for Dye Removal — **Jie Gao**, Zhiwei Thong, Kaiyu Wang, Neal Tai-Shung Chung

**Paper 376as:** Zero Valent Iron Nps Impregnated UF Membrane for Nitrobenzene Reduction and Fluoride Rejection — **Mihir K. Purkait**, Piya Mondal

**Paper 376at:** Organic Solvent Nanofiltration (OSN) Membranes Made from Plasma Grafting of Polyethylene Glycol on Cross-Linked Polyimide Ultrafiltration Substrates — **Zhuo Fan Gao**, Gui Min Shi, Yue Cui, Tai-Shung Chung

**Paper 376au:** Hydrophilic ZSM-5 Zeolite Membrane for Forward Osmosis — **Motomu Sakai**, Masahiko Matsukata

**Paper 376av:** Gas Separation Performance of Polymer-Ionene Hybrids — **Kathryn E. O'Harra**, Grayson P. Dennis, Jason E. Bara

**Paper 376aw:** Mitigation of Bidirectional Solute Flux Via Membrane Surface Coating of Zwitterion Functionalized Carbon Nanotubes in Forward Osmosis Process — **Shiqiang Zou**, Ethan D. Smith, Stephen M. Martin, Zhen He

**Paper 376ax:** Hydrosilylation-Based UV-Curable PDMS Pervaporation Membranes for *N*-Butanol Recovery — **Ju Yeon Lee**, Seon Oh Hwang, Soon Jin Kwon, Hyeon Kwon, Jung-Hyun Lee

**Paper 376ay:** Removal of Antibiotics Using Polyethylenimine Cross-Linked Nanofiltration Membranes: Relating Membrane Performance to Surface Charge Characteristics — **Shanshan Zhao**

**Paper 376az:** A Thin Film Composite Membrane Prepared from Monomers of Guaiaacol and Trimesoyl Chloride for Organic Solvent Nanofiltration — **Wei Li**, Ayang Zhou, Jinli Zhang

**Paper 376ba:** Preparation and Characterization of Graphene Oxide-Based Nanofiltration Membranes for Water Desalination — **Proggia Chirontoni**

**Paper 376bb:** Gas Transport Properties of Polysulfone Mixed-Matrix Membranes Embedded with Hexamethylenetetramine Dicyanamide Cadmium Nanoparticles — **Hossein Riazi**, Ahmad Arabi Shamsabadi, Morteza Sadeghi, Elmira Tavasoli, Masoud Soroush

**Paper 727c:** Bimetallic Nanoparticles Composite Poly(acrylic acid) Membrane for Water Remediation: Synthesis, Advance Characterization and Reactive Properties — **Hongyi Wan**, Nicolas Briot, M. S. Islam, Anthony Saad, Lindell Ormsbee, Dibakar Bhattacharyya

**Paper 752g:** Brackish Water Desalination with a Novel Polymer Nanocomposite Membrane — **Liliana R Villanueva**



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.

**(342) Fundamentals of Interfacial Phenomena II****Tuesday, Oct 30, 12:30 PM**

Omni William Penn Hotel, Conference Center A

Gerold A. Willing, Chair  
Clint P. Aichele, Co-Chair**Sponsored by:** Interfacial Phenomena**12:30 Paper 342a:** Hydrodynamics and Conjugate Mass Transfer from a Translating Spherical Droplet in a Continuous Phase — **Azeddine Rachih**, Dominique Legendre, Eric Climent, Sophie Charton**12:46 Paper 342b:** Molecular Modeling of Hydrophobins Near Interfaces Involving Gas, Oil and Water — **Andres Vodopivec**, Francisco R. Hung, Yuwu Chen, Paul Russo**1:02 Paper 342c:** Aging Oil-Water Interfaces with Asphaltene Adsorption: Interface Rheology and Heterogeneity — **Chih-Cheng Chang**, Arash Nowbahar, Vincent Mansard, Ian Williams, Todd M. Squires**1:18 Paper 342d:** Ordered Mesoporous Organosilica Materials with Systematically Controlled Surface Polarity — **Hyunjin Moon**, Songi Han, Susannah L. Scott**1:34 Paper 342e:** Magnetic Surfactant Surface Tension Functionality Vs. Magnetic Field Gradients — **Derek Reed**, Emily Koehler, Rachel Stanhope, Alex Fortenberry, Adam E. Smith, Paul Scovazzo**1:50 Paper 342f:** Molecular-Level Order Modulates the Hydrophobic Interactions between Nonpolar Self-Assembled Monolayers — **Bradley C. Dallin**, Hongseung Yeon, Chenxuan Wang, Nicholas L. Abbott, Reid C. Van Lehn**2:06 Paper 342g:** Assembly of Novel Tripeptides Hydrogels — **Lavenia Thursch**, Nicolas J. Alvarez, David DiGuiseppi, Reinhard Schweitzer-Stenner, Giuseppe Palmese**2:22 Paper 342h:** Probing Self-Assembly and Mechanical Properties of a Self-Assembled Molecular Gel — **Seyyed Meysam Hashemnejad**, Md Masrul Huda, Neeraj Rai, **Santanu Kundu****2:38 Paper 342i:** Hydrodynamics of Flash Evaporation of a Stagnant Liquid Column Under a Low Depressurization Rate — **Kush Kumar Dewangan**, Prasanta Kumar Das**(343) Industrial Applications in Design and Operations****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 409

Pieter Schmal, Chair  
Vijay Gupta, Co-Chair**Sponsored by:** Computers in Operations and Information Processing**12:30 Paper 343a:** The Industrial Implementation of Validated Dynamic Simulation and Optimisation Tools Towards Superior Beer Fermentation — **Alistair D. Rodman**, Megan Weaser, Lee Griffiths, Dimitrios I. Gerogiorgis**12:49 Paper 343b:** From Academia to Industry: Optimization Models for Shale Gas Development — **Markus G. Drouven**, Ignacio E. Grossmann**1:08 Paper 343c:** Reconciling Ranking Criteria with Fuzzy Sets for Effective Use in Project Portfolio Selection — **Scott J. Bury**, Satyajith Amaran, Sreekanth Rajagopalan, Anshul Agarwal**1:27 Paper 343d:** Multi-Scale Modeling and Design Optimization of an Industrial Hydrogen Production Plant with High-Resolution PSA and Steam-Methane Reformer Models — **Calvin Tsay**, Ankur Kumar, Thomas F. Edgar, Michael Baldea**1:46 Paper 343e:** Optimization of Circuitry Arrangements for Heat Exchangers — **Nikolaos Ploskas**, Christopher Laughman, Arvind Raghunathan, Nick Sahinidis**2:05 Paper 343f:** An Integrated Data-Driven Modeling & Global Optimization Approach for Production Planning Under Uncertainty — **C. Doga Demirhan**, Fani Boukouvala, William W. Tso, Kyungwon Kim, Hyeju Song, Efstratios N. Pistikopoulos**2:24 Paper 343g:** Robust Multi-Period Vehicle Routing: Construction of Uncertainty Sets and Evaluation Via Rolling-Horizon Simulations — **Anirudh Subramanyam**, José Miguel Láinez-Aguirre, Jose M. Pinto, **Chrysanthos E. Gounaris****2:43 Paper 343h:** Data-Driven Modelling and Optimization of Compressor Operations — **Harsha Nagesh Rao**, Harsha Vardhan Reddy Guddeti, Vikas Singh Bisen, **Iftekhhar A. Karimi**, Farooq Shamsuzzaman**(344) In Honor of Neal Chung III: Novel Membranes and Processes****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 304

Wanqin Jin, Co-Chair  
Xianshe Feng, Co-Chair  
Ranil Wickramasinghe, Co-Chair**Sponsored by:** Membrane-Based Separations**12:30 Paper 344a:** My Membrane Research at National University of Singapore (NUS) — **Neal Tai-Shung Chung****1:00 Paper 344b:** Novel Membranes, Membrane Processes and Membrane Devices — **Kamalesh K. Sirkar****1:20 Paper 344c:** Tuning the Interlayer Channels of GO Membranes for Molecule or Ion Transport — **Wanqin Jin****1:40 Paper 344d:** Catalytic Membranes for Biomass Hydrolysis and Dehydration — **S. Ranil Wickramasinghe**, Xianghong Qian**2:00 Paper 344e:** A Non-Thermal Process to Extract Aroma Compounds from Coffee Using Membranes — **Jennifer Du**, Gil Francisco, Kang Hu, **Xianshe Feng****2:20 Paper 344f:** Advancing Water Remediation Technologies By Nanostructured Membranes (invited paper) — **Dibakar Bhattacharyya**, Hongyi Wan, Lindell Ormsbee, Ashish Aher, Anthony Saad**2:40 Paper 344g:** Bioinspired Membranes and Membrane Processes — **Hong Wu**, Yanlei Su, Fusheng Pan, **Zhongyi Jiang****(345) In Honor of the 2017 Recipient of the Warren K. Lewis Award (Invited Talks)****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 412

Jeffrey J. Sirola, Chair  
Venkat Venkatasubramanian, Co-Chair**Sponsored by:** Education**12:30** Introductory Remarks**12:35 Paper 345a:** Rex's Role in Diversifying CACHE — **Warren D. Seider****12:55 Paper 345b:** School Head: Building for the Future — **Phillip C. Wankat****1:15 Paper 345c:** Continuous Processing Educational Modules — **Marianthi Ierapetritou****1:35 Paper 345d:** From Boilmakers to Tigers: Impact on a Career — **Selen Cremaschi****1:55 Paper 345e:** Developing the Process Systems Engineering Journal of Record — **Rafiqul Gani****2:15 Paper 345f:** Applications of Operations Research Methods — **Ignacio E. Grossmann****2:35 Paper 345g:** Reflections on a Unique Educator — **Doraismwami Ramkrishna****2:55** Concluding Remarks**(346) Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 316

Yuan Yao, Chair  
David R. Shonnard, Co-Chair**Sponsored by:** Sustainable Biorefineries**12:30 Paper 346a:** Carbon Footprint Analysis of Gasoline and Diesel from Forest Residues and Algae Using Integrated Hydrolysis and Hydroconversion Plus Fischer-Tropsch — **Olumide Winjobi**, Hossein Hossein Tavakoli, Bethany Klemetsrud, Robert Handler, Terry Marker, Michael Roberts, David R. Shonnard**12:55 Paper 346b:** Life Cycle Assessment of Bioenergy Oilseed Crops Produced in Rotation with Dryland Cereals in the Inland Pacific Northwest — **Sharath Ankathi**, Dan S. Long, Hero Gollany, David R. Shonnard**1:20 Paper 346c:** Evaluation of Environmental Tradeoffs of Producing Renewable Jet Fuel and Polyisoprene from Biomass — **Bahar Riazi**, Mukund Karanjikar, Sabrina Spatari**1:45 Paper 346d:** Life Cycle Assessment of Forest Biomass Energy Pathways in the Northeast US — **Ryan J. Quinn**, HakSoo Ha, Rohit Bhonagiri, Timothy A. Volk, Tristan Brown, Diane Kiernan, Robert Malmsheimer, Marie-Odile Fortier**2:10 Paper 346e:** Life Cycle Analysis As an Assessment Tool to Compare Process Alternatives — **Jaykumar Mavani**, Jorge E. Gatica, Michel Kahwaji Janho, Mauricio Colombo, Fernando Daniel Mele, María Rosa Hernández

**(347) Lignin for Sustainable Industrial Uses****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 325

Manju Misra, Chair  
Amar K. Mohanty, Co-Chair**Sponsored by:** Forest and Plant Bioproducts Division**12:30 Paper 347a:** Experimental and Computational Studies of Interfacial Interactions of Lignin Dimers with Lipid Bilayers — **Mahsa Moradipour, Xinjie Tong, Poorya Kamali, Shadrack O. Asare, Bert C. Lynn, Dorel Moldovan, Stephen E. Rankin, Barbara L. Knutson****12:55 Paper 347b:** Exploring Antimicrobial Properties of Lignin Derived Compounds and Materials — **Ryan Kalinoski****1:20 Paper 347c:** Fractionation of Kraft Lignin By Solvent Extraction and Exploration for Their Value-Added Applications — **Hao Li, Chunli Li, Jingjing Du****1:45 Paper 347d:** 3D Printing of Modified PA11 and Biocomposites: Processing and Performance Evaluation — **Manju Misra, Andrew Anstey, Claire Benwood, Amar K. Mohanty****2:10 Paper 347e:** Biodiesel As a Green Solvent to Improve the Dilute Acid Pretreatment of Lignocellulosic Biomass — **M.Ajaz Ahmad, Ayyaz Ahmad, Mahboob Ahmed Aadil, Teran Hilares Ruly****(348) Rising to the Challenge: Successful Leadership in Uncertain Times****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 331

Fernando Aguirre, Chair  
George Newcomb, Co-Chair  
Joseph Cramer, Co-Chair**Sponsored by:** Management Division**12:30** Introductory Remarks**12:35 Paper 348a:** Leading Engineering through Company Transformation — **Gayle Gibson****1:25 Paper 348c:** Merger...What...Who? — **Markus Scheller****1:50 Paper 348d:** Historic Department of Energy Site Transformed to a Private Sector Industrial Park — **Kenneth Rueter****2:15 Paper 348b:** Panel Discussion: Gayle Gibson, Ken Rueter, and Markus Scheller — **Gayle Gibson, Kenneth Rueter, Markus Scheller****(349) Microfluidic and Nanoscale Flows: Multiphase Systems and External Fields****Tuesday, Oct 30, 12:30 PM**

Omni William Penn Hotel, Frick

Aditya S. Khair, Chair  
Ya-Wen Chang, Co-Chair**Sponsored by:** Fluid Mechanics**12:30 Paper 349a:** Bubble-Bubble Dynamics Examined Using Microfluidic Channels — **Sibani Lisa Biswal****1:00 Paper 349b:** Hydrodynamic Interactions of Elastic Capsules in a Square Microfluidic Channel — **Abdollah Koolivand, Panagiotis Dimitrakopoulos****1:15 Paper 349c:** Microfluidic Micropipette Aspirator for Large-Scale Mechanical Characterization of Cells — **Shamim Ahmed, Siva A. Vanapalli****1:30 Paper 349d:** Microfluidic Device to Measure Blood Health — **Sarah E. Mena, Kevin R. Ward, Mark A. Burns****1:45 Paper 349e:** Generating Mono-Dispersed Femto/Pico-Liter Aqueous Droplets without External Oil Flow: AC Electrospray of Micro/Nanoemulsion — **Hsueh-Chia Chang, Zehao Pan, Yongfan Men, Satyajyoti Senapati****2:00 Paper 349f:** Migration and Concentration of DNA within Microfluidic Channels — **Ryan J. Montes, Anthony J.C. Ladd, Jason E. Butler****2:15 Paper 349g:** Convective Flows Driven By Solute Gradients in Microfluidic Channels — **Yang Gu, Varun Hegde, Kyle J. M. Bishop****2:30 Paper 349h:** Tears of Wine — **Prerana Rathore, Chenxian Xu, Vivek Sharma****2:45 Paper 349i:** Enhanced Dissolution of Liquid Microdroplets Under Planar Extensional Flow — **Adil Mustafa, Ahmet Erten, Oguz Kayilioglu, Aysenur Eser, Mustafa Eryurek, Muhammad Irfan, Metin Muradoglu, Melikhan Tanyeri, Alper Kiraz****(350) Microreaction Engineering I****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 404

Kishori T. Deshpande, Chair  
Simon Kuhn, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**12:30 Paper 350a:** Runaway in MICRO-Channel Reactors — **Sunjeev Venkateswaran, Benjamin Wilhite, Costas Kravaris****12:50 Paper 350b:** Cyclohexanone Ammoxidation over TS-1 Catalyst without Organic Solvent in a Microreaction System — **Yunpeng Hu, Dong Chen, Tao Wang Sr., Guangsheng Luo****1:10 Paper 350c:** Modeling-Aided and Experimental Approaches for Design of Microreactors Using 3D Printing — **Haomiao Zhang, Klavs F. Jensen****1:30 Paper 350d:** A Study on Catalytic Combustion of Methanol-Air Mixture in Microreactors — **Neha Yedala, Niket S. Kaisare****1:50 Paper 350e:** Nanoemulsion Meets Droplet Microfluidics: Controlled Mass Transport and Applications in Micro- and Nanoparticle Preparation — **Tonghan Gu, Fan He, Yunfei Zhang, T. Alan Hatton, Saif A. Khan****2:10 Paper 350f:** Process Intensification of Sulfuric Acid Alkylation Using a Microstructured Chemical System — **Liantang Li, Jisong Zhang, Chencan Du, Guangsheng Luo****2:30 Paper 350g:** Single-Droplet Flow Chemistry Platform for High-Throughput Studies of Rhodium-Catalyzed Hydroformylation Reactions — **Cheng Zhu, Keshav Raghuvanshi, Connor W. Coley, Milad Abolhasani****(351) Molten Salt Applications for Heat Transfer and Nuclear Reactors****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 326

Raluca Scarlat, Chair

**Sponsored by:** Nuclear Engineering Division**12:30 Paper 351a:** Development of an Infrared Measurement Method for Molten Fluoride Salt — **Will B. Derdeyn, Alireza Shahsafi, William Mueting, Mikhail A. Kats, Raluca Scarlat****12:50 Paper 351b:** Density Measurement of Molten Fluoride Salts — **Ricardo Vidrio****1:10 Paper 351c:** Design and Operation of Batch Fluoride Salt Purification Systems — **Kevin Robb****1:30 Paper 351d:** Modeling Radiative Heat Transfer in High-Temperature Liquid-Salts — **Carolyn Coyle, Emilio Baglietto, Charles W. Forsberg****1:50 Paper 351e:** Viability of Molten Salt Reactors for the Production of Molybdenum-99 — **Michael Stoddard, John Harb, Matthew Memmott****2:10 Paper 351f:** Compatibility of Ni-Cr Alloys in Static and Flowing Commercial Molten Chloride Salt — **Bruce Pint, Stephen Raiman****2:30 Paper 351g:** Investigating Chromium Dealloying in Molten Chloride Salt — **Stephen Raiman, Richard Mayes, Jake McMurray, Jisue Moon****(352) Novel Nanostructured Catalytic Materials II****Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 403

Chao Wang, Chair  
Michael M. Nigra, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**12:30 Paper 352a:** Dry Reforming of Methane over  $\text{Ce}_{0.7}\text{Ti}_{0.3}\text{O}_{2-x}$  supported Nickel Catalyst — **Sachin Nandanwar, Yunkai Zou, Linze Du, Joseph H. Holles, Jing Zhou****12:50 Paper 352b:** Controlled Metal@Metal Oxide Core-Shell Structures for Selective Heterogeneous Catalysis — **Bingwen Wang, Jing Zhang, J. Will Medlin, Eranda Nikolla****1:10 Paper 352c:** Protecting the Fe Active Phase from Oxidation Under Hydrodeoxygenation Conditions: Evaluating the Influence of Promoters and External Electric Fields — **Jacob Bray, Alyssa Hensley, Greg Collinge, Jean-Sabin McEwen****1:30 Paper 352d:** Synthesis and Catalytic Testing of Lewis Acidic Nano-MFI Zeolites for Epoxide Ring Opening Reaction with Alcohol — **Aamena Parulkar, Rutuja Joshi, Nitish Deshpande, Alexander Spanos, Nicholas Brunelli****1:50 Paper 352e:** Understanding Intramolecular Cooperativity in Acid-Base Silica-Supported Organocatalysts — **Jingwei Xie, Nathan Ellebracht, Christopher W. Jones****2:10 Paper 352f:** Study of Ethanol Decomposition Mechanism over Combustion Synthesized Bimetallic Cu-Co Nanoparticles — **Anand Kumar, Anchu Ashok, Faris Tarlochan****2:30 Paper 352g:** Synergetic Effect of Ultrafine NiCo Bimetallic Alloy Nanoparticles Derived from Bimetal-Organic Frameworks — **Huanjun Wang, Xiaodan Li II, Xiaocheng Lan III, Tiefeng Wang**



### (353) Nucleic Acid Materials and Delivery

**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 328

Forrest Kievit, Co-Chair  
Lorraine Leon, Co-Chair

**Sponsored by:** Biomaterials

**12:30 Paper 353a:** Novel, Stimuli-Responsive Hydrogels Utilizing Ionic Interactions for the Controlled and Targeted Delivery of Nucleic Acid Nanospheres to Prevent Secondary Cataracts — **Mark E. Byrne**, Laura L. Osorno, Robert Getts, Mindy George-Weinstein

**1:06 Paper 353b:** miR233-Loaded Immunomodulatory Adhesives for the Treatment of Chronic Wounds — **Bahram Saleh**, Harkiran Dhaliwal, Roberto Portillo Lara, Ehsan Shirzaei Sani, Mansoor Amiji, Nasim Annabi

**1:24 Paper 353c:** Lipid Nanoparticle-Mediated Delivery of Chemically Modified mRNA Significantly Enhances Protein Expression in Mice — **Khalid A. Hajj**, Kathryn A. Whitehead

**1:42 Paper 353d:** Effect of Polyplex Charge on Cellular Internalization and Gene Expression — **Landon A. Mott**, Caleb Akers, Daniel W. Pack

**2:00 Paper 353e:** Characterization of Daunomycin Binding Affinity Toward Specifically Engineered DNA Sequences to Modulate Behavior of Nanoscale Drug Delivery Vehicles — **Robert Mosley**, Ricky J. Whitener, Jacek Wower, Mark E. Byrne

**2:18 Paper 353f:** Dynamic, Reversible Control of Hydrogel Stiffness Using DNA Crosslinkers — **Nicholas Stephanopoulos**

**2:36 Paper 353g:** Physically Crosslinked DNA-Based Injectable Hydrogels for Bone Regeneration — **Sayantani Basu**, Settimio Pacelli, Arghya Paul

### (354) Particulate and Multiphase Flows: Particle and Suspension Dynamics

**Tuesday, Oct 30, 12:30 PM**

Omni William Penn Hotel, Phipps

David T. Leighton Jr., Chair  
Vivek Narsimhan, Co-Chair

**Sponsored by:** Fluid Mechanics

**12:30 Paper 354a:** Transport and Dispersion of Active Particles in Porous Media — **Roberto Alonso-Matilla**, Brato Chakrabarti, Antoine Beringer, David Saintillan

**1:00 Paper 354b:** Non-Equilibrium Deformation and Relaxation of Giant Floppy Vesicles in a Precisely Controlled Extensional Flow — **Dinesh Kumar**, Charles M. Schroeder

**1:15 Break**

**1:30 Paper 354d:** Taylor-Couette Flows of Suspensions — **Madhu V Majji**, Sanjoy Banerjee, Jeff Morris

**1:45 Paper 354e:** Theory for Flow-Induced Particle Segregation in Suspension Flows — **Rodrigo Reboucas**, Michael Loewenberg

**2:00 Paper 354f:** Collective Effects in the Sedimentation of Particles in Viscoelastic Fluids — **William L. Murch**, Sreenath Krishnan, Eric S. G. Shaqfeh

**2:15 Paper 354g:** Sphere Sedimentation in Wormlike Micelles: Effect of Micellar Relaxation Spectrum and Gradients in Micellar Extensions — **Shijian Wu**, Hadi Mohammadigoushki

**2:30 Paper 354h:** Drilling Fluids and Mechanisms of Particle Sedimentation — **Manizheh Ansari**, Dinesh V. Kalaga, Damon Turney, Robert J. Messinger, Sanjoy Banerjee, Masahiro Kawaji

**2:45 Paper 354i:** Lateral Migration and Sorting of Elastic Capsules in Microfluidic Devices — **Abdollah Koolivand**, Panagiotis Dimitrakopoulos

### (355) Photovoltaic Materials and Devices

**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 330

Aaron T. Fafarman, Chair

**Sponsored by:** Electronics and Photonics

**12:30 Paper 355a:** *Invited:* Impact of Crystallographic Orientation Disorders on Electronic Heterogeneities in Metal Halide Perovskite Thin Films — **Benjamin Foley**, Seung-Hun Lee, Kai Xiao, Benjamin Doughty, Ying-Zhong Ma, Joshua Choi

**12:55 Paper 355b:** Enhancing Efficiency and Stability of Triple-Cation, Double-Halide Pb-Sn Alloyed Perovskite Solar Cells — **Qiuming Yu**, Gabriella Tosado, Yi-Yu Lin, Erjin Zheng

**1:15 Paper 355c:** Effect of Alloying on the Thermodynamic Stability and Optoelectronic Properties of Cesium Lead Halide Perovskites — **Aaron T. Fafarman**

**1:35 Paper 355d:** Composition-Dependent Ultrafast Carrier Dynamics in  $\text{Cu}_2\text{ZnSnSe}_4$  Single Crystals — **Siming Li**, Michael A. Lloyd, Hannes Hempel, Charles J. Hages, José Márquez, Andrew A. Golembeski, Thomas Unold, Rainer Eichberger, Brian E. McCandless, Jason B. Baxter

**1:55 Paper 355e:** Absorptive Spectral Control for High-Efficiency Thin-Film Thermophotovoltaics — **Tobias Burger**, Dejiu Fan, Kyusang Lee, Stephen Forrest, Andrej Lenert

**2:15 Paper 355f:** Titanium Oxide Hydrates As Optically and Photonically Versatile Species in Inorganic-Organic Hybrids for Polymer-Based Energy Harvesting and Conversion Devices — **Alex Balzer**, Ilaria Bargigia, Stefan Bachevillier, Artem Levitski, Gitty Frey, Carlos Silva, Natalie Stingelin

**2:35 Paper 355g:** Mechanically Robust Organic Photovoltaics Using Thiol-Ene Interpenetrating Networks — **Jorge Mok**, Zhiqi Hu, Changxu Sun, Rodrigo Munoz, Joshua Jackson, Rafael Verduzco

### (356) Polymers in Additive Manufacturing

**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 333

Mingjiang Zhong, Chair  
Michael J. Bortner, Co-Chair

**Sponsored by:** 3D Printing

**12:30 Paper 356a:** Tough, High Impact Resistant 3D Printed Objects from Core-Shell Filaments — **Bryan D. Vogt**, Fang Peng, Miko Cakmak

**1:00 Paper 356b:** Solution-Based 3D Printing of Hierarchical Porous Polymers — **Fengyi Zhang**, Yao Ma, Jianshan Liao, Victor Breedveld, Ryan Lively

**1:20 Paper 356c:** 3D Printing with Soft Porous Silicones By the Homocomposite Thixotropic Paste (HTP-3DP) Method — **Sangchul Roh**, Orlin D. Velev

**1:40 Paper 356d:** Additive Manufacturing of Polypropylene/Hydrogenated Resin Blends: Effect on Crystallinity, Morphology and Mechanical Properties — **Arit Das**, Alexandra Marnot, Eugene Joseph, Michael J. Bortner

**2:00 Paper 356e:** Filament Extension Atomizer: Novel Aerosol Generation from Polymer Melts and Applications in Additive Manufacturing — **Jerome Unidad**, Kathryn Murphy, Scott Solberg, David Johnson

**2:20 Paper 356f:** 3D Printing of Hydrogels with Spontaneous Formation of Solvent-Induced Patterns — **Chya-Yan Liaw**, Jorge Pereyra, Murat Guvendiren

### (357) Polymers in Industry - Rising Stars (Invited Talks)

**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 327

Blair Kathryn Brettmann, Chair  
Ibrahim A. El-Hedok, Co-Chair

**Sponsored by:** Polymers

**12:30 Paper 357a:** *Silicon-Based Xpl Film* That Mimics Healthy Skin and Effectively Improves Skin Hydration; And *Elite Fiber* That Delivers Heat Sensitive Biologics in a Sustained Manner — **Alpesh Patel**

**12:55 Paper 357b:** Rheological Studies of Poly (DL-lactic acid) Solutions and Melts — **Xue Chen**, Chulwoo Jung, Ronald G. Larson

**1:20 Paper 357c:** Rheology of Particle-Laden Polymeric Fluids: A Perspective from Mixing Orders — **Hao Sun**

**1:45 Paper 357d:** The Spectacular Properties of Porous  $\beta$ -Cyclodextrin Polymers — **Alaaeddin Alsaiee**

**2:10 Paper 357e:** Studies to Gain New Insights into Emulsion Polymerization and Optimization to Produce Novel Paper Coatings Technologies — **Bryan L. McCulloch**

### (358) Population Balance Modeling for Particle Formation Processes: Nucleation, Aggregation and Breakage Kernels

**Tuesday, Oct 30, 12:30 PM**

David L. Lawrence Convention Center, 414

Dana Barrasso, Chair  
R. Bertrum Diemer Jr., Co-Chair

**Sponsored by:** Particle Production and Characterization

**12:30 Paper 358a:** Global System Analysis of Twin Screw Granulation Using Population Balance Modelling in gPROMS — **Li Ge Wang**, Dana Barrasso, David Slade, James D. Litster

**12:55 Paper 358b:** Effect of Crystal Size on the Breakage of High Aspect Ratio Crystals in Stirred Slurries — **Priscilla J. Hill**

**1:20 Paper 358c:** Fundamental Prediction of Agglomeration and Entrainment Rates for Cohesive Powders in a Riser Flow — **Kevin M. Kellogg**, Peiyuan Liu, Casey LaMarche, Christine M. Hrenya



**1:45 Paper 358d:** Molecules As Building Blocks in a Novel Population Balance Model for Flash Nano-Precipitation: Investigation of the Different Good Solvents Effect on Nanoparticle Formation — **Alessio D. Lavino, Marco Ferrari, Daniele Marchisio**

**2:10 Paper 358e:** Distribution Reconstruction from Moments Via Orthogonal Polynomials — **R. Bertrum Diemer Jr.**

**2:35 Paper 358f:** Modeling of Breakage Process Using Monte Carlo Simulations in Spray Fluidized Bed Granulator — **Ashok Das, Jitendra Kumar**

### (359) Predictive Control and Optimization I

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 408

Jin Wang, Chair  
Xiaonan Wang, Co-Chair

**Sponsored by:** Systems and Process Control

**12:30 Paper 359a:** Optimization-Based Predictive Control of Networked Process Systems with Discrete and Delayed Sensor-Controller Communication — **Da Xue, Nael H. El-Farra**

**12:49 Paper 359b:** Stochastic-Tube MPC for Offset-Free Tracking in the Presence of Plant-Model Mismatch — **Joel Paulson, Tito Santos, Ali Mesbah**

**1:08 Paper 359c:** An Efficient Distributed Algorithm for Multistage Scenario Model Predictive Control Using Primal Decomposition — **Dinesh Krishnamoorthy, Eka Suwartadi, Sigurd Skogestad, Johannes Jäschke**

**1:27 Paper 359d:** Approximate Dynamic Programming Based Control of Hydraulic Fracturing Process to Achieve Uniform Proppant Concentration Level — **Harwinder Singh Sidhu, Prashanth Siddhamshetty, Abhinav Narasingam, Joseph Sangil Kwon**

**1:46 Paper 359e:** Advanced-Step Multistage Nonlinear Model Predictive Control — **Zhou (Joyce) Yu, Lorenz T. Biegler**

**2:05 Paper 359f:** Decomposition of Optimization Problems Using Community Detection and Its Application in Nonlinear Model Predictive Control — **Wentao Tang, Andrew Allman, Davood Babaei Pourkargar, Prodromos Daoutidis**

**2:24 Paper 359g:** Safeness Index-Based Economic Model Predictive Control of Stochastic Nonlinear Systems — **Zhe Wu, Helen Durand, Panagiotis D. Christofides**

**2:43 Paper 359h:** Dual Offset Blocking Strategy for Computationally-Efficient Model Predictive Control — **Sang Hwan Son, Jong Min Lee**

### (360) Process Intensification By Enhanced Heat and Mass Transfer

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 335

Kishori T. Deshpande, Chair  
Daniela Ferrari, Co-Chair  
Robert Broekhuis, Co-Chair

**Sponsored by:** Process Intensification & Microprocess Engineering

**12:30 Paper 360a:** Study of Local Boiling Heat Transfer for Micro Nano Surface Structures Using a 3D Transient Heat Conduction Model — **Hao-Ran Lu, Ya-Qiao Wang, Dong-Chuan Mo, Yuan-Xiang Fu, Shu-Shen Lyu, Yi Heng**

**12:50 Paper 360b:** Novel Adsorption-Based Separation Technology for Gas Treating Applications — **Phillip K. Schoch, Rodrigo Blanco-Gutierrez, Bennett D. Marshall, Justin Federici, Chien-Chiang Chen, Tracy Fowler, Patrick McMahon**

**1:10 Paper 360c:** Process Intensification, a Promising Approach in Separating a Ternary System Using Distillation to Reduce Energy Consumption: Case Study — **Ameen AlGhamdi, Jagan Mohan Rallapalli**

**1:30 Paper 360d:** Improved Fixed-Bed Transport Characteristics: A Shortcut Method to Optimize Catalyst Pellet Specifications — **Alexander Pietschak, Markus Kaiser, Hannsjörg Freund**

**1:50 Paper 360e:** Multi-Material, Microchannel Heat Exchanger Design for Enhanced Heat Exchange Processes By Anisotropic Conduction — **Lucas Freiberg, Matthew Young Cobylin, Nick AuYeung, Goran Jovanovic**

**2:10 Paper 360f:** Small-Scale Production of Platform Chemicals from Coal with Low-Temperature Microwave Plasma — **George Skoptsov, Kurt Zeller, Randy Vander Wal**

**2:30 Paper 360g:** Effectiveness Factor Phenomena for the Transition between PBR (Packed Bed Reactor) and MR (Membrane Reactor) Via Coupled Heat and Mass Transfer — **Secgin Karagoz, Theo Tstosis, Vasilios Manousiouthakis**

### (361) Protein Structure, Function, and Stability

**Tuesday, Oct 30, 12:30 PM**  
Westin Convention Center, Westmoreland East

James Van Deventer, Chair  
Amy J. Karlsson, Co-Chair  
Yongchan Kwon, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 361a:** Structural Studies of a Cyanobacterial Bicarbonate Uptake Regulator — **Brent L. Nannenga, Guan hong Bu, David R. Nielsen**

**12:48 Paper 361b:** Biophysical Characterization Platform for AAV-Based Gene Therapy Products — **Zifan Gong, Arun Alphonse Ignatius**

**1:06 Paper 361c:** Computational High-Throughput Screening of Modified RNA Interactions with Proteins — **Asuka A. Orr, Juan Camilo Gonzalez, Lydia M. Contreras, Phanourios Tamamis**

**1:24 Paper 361d:** Flap-Opening Dynamics and Ligand Unbinding of HIV-1 Protease Studied Using Accelerated MD Simulations — **Jasmine Gardner, Cameron F. Abrams**

**1:42 Paper 361e:** Catechin-Mediated Toxin Unfolding As an Antivirulence Strategy — **Angela C. Brown, En-Hyung Chang**

**2:00 Paper 361f:** Expression of EK Fusion Proteins to Enhance Protein Kinetics and Stability — **Erik J. Liu, Shaoyi Jiang**

**2:18 Paper 361g:** Protein Folding, Misfolding and Aggregation in Amyloid Disease — **Regina M. Murphy**

### (362) Refining and Petrochemical Plant Modelling and Operations Improvements II

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 323

Vladimir Mahalec, Chair  
Wenli Du, Co-Chair  
Mark Darby, Co-Chair

**Sponsored by:** Fuels and Petrochemicals Division

**12:30 Paper 362a:** Virtual Manufacturing System for Refinery Process — **Xiaoqiang Wang, Wenli Du, Weimin Zhong, Minglei Yang, Jian Long, Chen Fan**

**12:51 Break**

**1:12 Paper 362c:** Radiative Heat Transfer Modeling Using Monte Carlo Techniques and CFD for Industrial Furnaces — **Abdulaziz AL-Arifi, Awais Ahmed, Adel Alghamdi, Ahmed AL-Khalaf, Aaron Vandeputte**

**1:33 Paper 362d:** Optimal Cleaning Scheduling and Control of Heat Exchanger Networks: An Industrial Case Study — **Federico Lozano Santamaria, Sandro Macchietto**

**1:54 Paper 362f:** Rigorous Thermodynamic Analysis of a Baseload LNG Chain with Different Boil-Off Gas Minimization Strategies — **Zineb Bouabidi, Mary Katebah, Mohamad Hussein, Abdulla Al-Hajri, Easa Al-Musleh**

### (363) Self and Directed Assembly at the Nanoscale I

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 311

Javen Weston, Chair  
Evan K. Wujcik, Co-Chair

**Sponsored by:** Nanoscale Science and Engineering Forum

**12:30 Paper 363a:** Directed Assembly of Polarizable Nanoparticles — **James Swan, Zachary Sherman**

**12:48 Paper 363b:** Electrochemical Etching and Oxidation Stability of Mxene Nanosheets — **Touseef Habib, Wanmei Sun, Smit Shah, Miladin Radovic, Micah J. Green**

**1:06 Paper 363c:** Modulation of Carrier Type in Nanocrystal-in-Matrix Composites By Interfacial Doping — **Richa Sharma, April M. Sawvel, Anna Llordes, Zhi Liu, Dennis Nordlund, Jeffrey Urban, Delia J. Milliron**

**1:24 Paper 363d:** Antigen-Antibody Nanoparticle Bioconjugates and Their Polymorphs — **Caroline Desgranges, Jerome Delhommele**

**1:42 Paper 363e:** Adsorption and Denaturation of Polymeric Nanoparticles at an Interface — **Chang Tian, Jie Feng, Robert K. Prud'homme**

**2:00 Paper 363f:** Nonclassical Nucleation of Tumor Suppressor p53 Fibrils Hosted By Mesoscopic Protein-Rich Clusters — **Mohammad Safari, Jacinta Conrad, Anatoly Kolomeisky, Peter Vekilov**

**2:18 Paper 363g:** Driving Forces for Oriented Aggregation-Based Crystallization and Assembly — **Xin Zhang, Yang He, Maria Sushko, Jia Liu, Langli Luo, James J. De Yoreo, Scott X. Mao, Chongmin Wang, Kevin Rosso**

**2:36 Paper 363h:** Rheo-Electric Behavior of Carbon Black Suspensions in Shear Flow — **Jeffrey J. Richards**, Julie Hipp, Norman Wagner

**(364) Special Session: Celebrating Career Accomplishments of Prof. Yutaka Tsuji (Invited Talks)**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 415

Toshitsugu Tanaka, Chair  
Takuya Tsuji, Co-Chair

**Sponsored by:** Fluidization and Fluid-Particle Systems

**12:30 Paper 364a:** Differentiated Research Strategy — **Yutaka Tsuji**

**1:15 Paper 364b:** DEM Simulation with Scaled-up Particles — **Kimiaki Washino**

**1:40 Paper 364c:** Multi-Scale Modeling of Reactive Dense Flows — **Kun Luo**

**2:05 Paper 364d:** Real-Time Magnetic Resonance Imaging of Dynamic 3D Granular Systems — **Christoph R. Müller**

**2:30 Paper 364e:** Insights and Model Development Enabled By DEM and CFD-DEM Simulations — **Sankaran Sundaresan**

**(365) Sustainable and Green Product Design**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 319

Sitaraman Krishnan, Chair  
Mu Wang, Co-Chair  
Kishori T. Deshpande, Co-Chair

**Sponsored by:** Product Design

**12:30 Paper 365a:** Carbon Dioxide Introduced for Green Synthesis of Thiuram Disulfides Vulcanization Accelerators Under Mild Conditions — **Jiayu Hu**, Kai Wang, Guangsheng Luo

**12:55 Paper 365b:** Plastic Waste Accumulation Problem and Emerging Solutions — **Wan-Ting Chen**, Nien-Hwa Linda Wang

**1:20 Paper 365c:** Process Systems Engineering: Limits of Performance of the “Cyclic” Waste Plastic Economy — **James A. Fox**, Baraka Celestin Sempuga

**1:45 Paper 365d:** Discovery of Electronics Cooling Fluids — **Yijia Sun**, Nick Sahinidis

**2:10 Paper 365e:** Computer-Aided Design of Products Derived from Biomass Pyrolysis — **Suela Jonuzaj**, Nilay Shah, Claire S. Adjiman

**2:35 Paper 365f:** Reactive Distillation Combined with Pervaporation for Biobased By-Product Recovery — **Daniela Painer**, Susanne Lux, Matthaeus Siebenhofer

**(366) The Food-Energy-Water Nexus**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 315

Vikas Khanna, Chair  
Yuan Yao, Co-Chair

**Sponsored by:** General

**12:30 Paper 366a:** Analysis of a Circular Economy: From Food Waste to Foods — **Jeremy Taylor**, Ross Lee, Tyler Casteel, Alyson Perez, Dan Spracklin, Justinus A. Satrio

**12:50 Paper 366b:** Re-Wiring the Domestic Food Trade for Reducing Irrigation Impacts in the United States — **Nemi Vora**, Colin P. Gillen, Oleg A. Prokopyev, Vikas Khanna

**1:10 Paper 366c:** Food, Energy, Fuels and Chemical Feedstocks from Rice Crops: Multi-Objective Optimisation of Multi-Product Value Chains for the Philippines — **Stephen S. Doliente**, Sheila Samsatli

**1:30 Paper 366d:** Modeling the Impacts of International Food Trade on Contaminant Transport and Human Exposure — **Megha Bedi**, Carla Ng

**1:50 Paper 366e:** Using Agricultural Wastes to Recover Rare Earth Elements from End-of-Life Materials — **David W. Reed**, Vicki S. Thompson, Yoshiko Fujita, Jacob Fisher, Michael Crain-Zamora, Yongqin Jiao

**2:10 Paper 366f:** Membranes for Nutrient Concentration, Industrial Separations and Applications Beyond — **Jie Song**, Jacob Moen

**(367) Thermophysical Properties and Phase Behavior**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 307

Sanket Deshmukh, Chair  
Clare McCabe, Co-Chair  
Erik E. Santiso, Co-Chair  
Hiroyuki Matsuda, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**12:30 Paper 367a:** Geometry, Confinement and Directed Colloid Motion — **Kathleen J. Stebe**

**1:08 Paper 367b:** Higher-Order Hydrophobic Effects: Capturing the Distinct Heat Capacity and Compressibility Signatures of Non-Polar Gas Hydration with Molecular Simulations — **Henry S. Ashbaugh**

**1:27 Paper 367c:** Electrostatic and Induction Effects in Solubility of Water in Alkane — **Dilip Asthagiri**, Arjun Valiya Parambathu, Walter G. Chapman

**1:46 Paper 367d:** Effect of Fluorination on Interfacial Properties and Partitioning of Alcohols — **Mohammad Barhaghi**, Chloe Luyet, Jeffrey J. Potoff

**2:05 Paper 367e:** Application of Kirkwood-Buff Integral Data in Development of a Charmm-Type Carbohydrate Force Field to Model Activity Behavior — **Theresa Cloutier**, Chaitanya Sudrik, Hasige Sathish, Bernhardt L. Trout

**2:24 Paper 367f:** Transitioning from Empirical to *Ab Initio* Potentials for the Prediction of Thermodynamic Properties and Phase Equilibria — **Richard J. Sadus**

**2:43 Paper 367g:** Constrained Subset Selection for the Regression of Multi-Component Helmholtz Energy Equations — **Marissa Engle**, Nick Sahinidis

**(368) The Use of CFD and Analysis Tools in Understanding of Mixing Processes**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 334

Justin Walker, Chair  
Minye Liu, Co-Chair

**Sponsored by:** North American Mixing Forum

**12:30 Paper 368a:** CFD Modeling of Turbulent Reactive Flows with Bourne Chemistry Comparisons — **Quan Yuan**, Paul A. Gillis, Sarat Chandra Kuchibhatla, Jim Pressler

**12:55 Paper 368b:** Validation of the Coalescence-Dispersion Model for Complex Chemical Reactions — **Gary K. Patterson**

**1:20 Paper 368c:** A Direct Numerical Simulation of a Marginally Turbulent Stirred Vessel Equipped with a Rushton Turbine — **Niall O'Byrnes**, Harry E.A. Van den Akker

**1:45 Paper 368d:** Blending of Miscible Fluids — **John A. Thomas**, Brian DeVincentis, Kevin Smith

**2:10 Paper 368e:** Deconstruction of Mixing Processes Using Computational Fluid Dynamics and Z-Transform — **De-Wei Yin**

**(369) Tutorial on the Catalyst Cost Estimation Tool: Economic Insight for Catalyst Synthesis and Scale-up Research I (Invited Talks)**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 406

Joshua Schaidle, Chair  
Frederick Baddour, Co-Chair  
Kurt Van Allsburg, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 369a:** Introduction to the Chemical Catalysis for Bioenergy Consortium — **Joshua A. Schaidle**

**12:40 Paper 369b:** Introduction to Catalyst Cost Estimation — **Frederick Baddour**

**1:00 Paper 369c:** Tutorial on the Catcost Tool: FCC Catalyst Example — **Kurt Van Allsburg**

**1:40 Break**

**1:55 Paper 369d:** Capability Highlight: A Simple Step Method for Processing Costs — **Frederick Baddour**

**2:15 Paper 369e:** Flow Synthesis: An Improved Path to Market for Nanoparticle Catalysts — **Noah Malmstadt**

**2:35 Paper 369f:** Capability Highlight: Estimation of Spent Catalyst Value — **Lesley J. Snowden-Swan**

**(370) Value-Added Chemicals from Natural Gas**

**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, 321

Dushyant Shekhawat, Chair  
Götz Vesper, Co-Chair  
John Hu, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**12:30 Paper 370a:** Methane and Ethane to High Value Products — Pushing Beyond Historical Paradigms — **John A. Sofranko**, Elena Y. Chung, Gary A. Sawyer, C. Andrew Jones

**12:47 Paper 370b:** Catalyst Development for Natural Gas Monetization — **Daniyal Kiani**, Sagar Sourav, Lohit Sharma, Israel E. Wachs, Jonas Baltrusaitis

**1:04 Paper 370c:** Catalytic Wall Reactor for Non-Oxidative Methane Conversion — *Su Cheun Oh, Dongxia Liu*

**1:21 Paper 370d:** Exploring Strategies to Improve Yields of Oxidative Coupling of Methane in a Chemical Looping System — *Deven Baser, Zhuo Cheng, Sourabh Nadgouda, Lang Qin, Liang-Shih Fan*

**1:38 Paper 370e:** Metal-Mediated Transient Hydrogen Scavenging for Enhanced Aromatics Yield during Non-Oxidative Methane Aromatization on Mo/H-ZSM-5 Catalysts — *Anurag Kumar, Aditya Bhan*

**1:55 Paper 370f:** Promotional Effect of Cr in Mo<sub>2</sub>C catalyst Supported on Sulfated Zirconia for Methane Dehydroaromatization — *Ashraf Abedin, Swarom Kanitkar, Srikar Bhattar, James J. Spivey*

**2:12 Paper 370g:** Engineering Fe-HZSM-5 for Methane Dehydroaromatization — *Yifan Deng, Yu-Chieh Cheng, Yahui Yang, Yungchieh Lai, Götz Vesper*

**2:29 Paper 370h:** Magnesium Vanadate Catalyzed Oxidative Dehydrogenation of Ethane to Ethylene Using CO<sub>2</sub> As a Soft Oxidant — *Chinmoy Baroi, Harry W. Rollins, Rebecca Fushimi*

**2:46 Paper 370i:** Chemical Looping for the Oxidative Cracking of Shale Condensates — *Luke Neal, Vasudev Pralhad Haribal, Fanxing Li*

**(371) WIC 20th Anniversary: Celebrating Women in Chemical Engineering II (Invited Talks)**  
**Tuesday, Oct 30, 12:30 PM**  
David L. Lawrence Convention Center, Spirit of Pittsburgh A

Julianne L. Holloway, Chair  
Ashlee N. Ford Versypt, Co-Chair  
Megan E. Donaldson, Co-Chair

**Sponsored by:** WIC 20th Anniversary: Celebrating Women in Chemical Engineering

**12:30 Symposium Introduction by WIC 20th Anniversary Symposium Chair,** Julianne Holloway

**12:32 Welcome and Introductory Remarks by AIChE Executive Director,** June Wispelwey

**12:45 Paper 371a:** Some Historical Information and Statistics on Women in Chemical Engineering and in AIChE — *Maria K. Burka*

**1:05 Paper 371b:** Modeling and Simulation of Complex Particle-Laden Flows — *Jennifer Sinclair Curtis*

**1:25 Paper 371c:** Computational Design of Peptides to Detect Human Health Biomarkers — *Carol Hall*

**1:45 Paper 371g:** Reflections from Four Decades of Collegiality, Collaboration and Competition in AIChE — *Alice P. Gast*

**2:05 Paper 371d:** Heterogeneous Catalyst Design at the Single Atom Limit for Efficient Chemicals Production — *Maria Flytzani-Stephanopoulos*

**2:25 Paper 371e:** Chemical Process Development – Even for Reaction Engineers, it Ain't Just Kinetics — *Cheryl Teich*

**2:45 Paper 371f:** Potential of the Bioproducts and Biofuels Bioeconomy — *Kimberly L. Ogden*

**(372) Poster Session: Chemical Engineering Education**

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Daniel Lepek, Chair  
Joshua A. Enszer, Co-Chair

**Sponsored by:** Education

**Paper 372a:** An Interactive Tool for Learning Spreadsheets — *Matthew Liberatore, Katherine Roach*

**Paper 372b:** The Emulsion Lab: An Industry Relevant Experiment for Senior Unit Operations — *Alex J. Bertuccio*

**Paper 372c:** Engaging Engineering Students Using Memes — *Kristine Horvat*

**Paper 372d:** Integrating Sustainability Principles into Chemical Engineering Core Courses: A PBL Approach — *Omar Movil-Cabrera, Ryan C. Johnson, Elba Herrera*

**Paper 372e:** Revolutionizing Engineering Education at Oregon State University — *Milo D. Koretsky, Susan Bobbitt Nolen, Michelle Bothwell, Christine Kelly, Susannah Davis, Devlin Montfort, Jim Sweeney*

**Paper 372f:** Collaborative Writing "Wiki Tool" in a Chemical Engineering Laboratory — *Daniel Knight*

**Paper 372g:** Developing Standards for an Operations Center Process Safety Educational Exercise Using Simulators — *Hayley Caddes, Matthew B. Garvey, Donald C. Glaser, Robert G. Bozic*

**Paper 372h:** Development of "Smart Materials" Master's Degree Program Module for Chemical Engineers — *Artem Bezrukov*

**Paper 372i:** The Link between Spatial Visualization and Chemical Engineering Problem-Solving — *Norman Loney*

**Paper 372j:** Photobioreactor Design and Biodiesel Synthesis — *Kyle Branch, Anthony Butterfield*

**Paper 372k:** Impact of Online Numerical Response Questions on Student Learning in Parallel Sections — *J Richard Elliott*

**Paper 372m:** Use of Numerical Software in Education and Research — *Mordechai Shacham, Michael B. Cutlip*

**Paper 372n:** A Fully Online Matlab Course for Freshman Chemical Engineers — *Aaron M. Drews*

**Paper 372o:** Social and Tactile Augmented Reality in an Undergraduate Chemical Engineering Laboratory — *Rainier Barrett, Heta Gandhi, Andrew White*

**Paper 372p:** Using Wiki Technology to Streamline Your ABET Portfolio — *Kevin Hadley, Kenneth M. Benjamin*

**Paper 372q:** A Web-Based Database-Driven Assessment Management Tool — *Andrew J. Schultz, Christine Human, David A. Kofke, Jeffrey R. Errington*

**Paper 372r:** 3D Printed Centrifugal Pump Impellers: A Unit Operations Experiment — *Thehaznman (Thihal) K. Ponnaiyan, Cory Zalesak, Glenn Lipscomb*

**Paper 372s:** Chemical Engineering Lab for Seniors at United States Military Academy — *Matthew Armstrong, Enoch Nagelli, Andrew Biaglow, Geoffrey Bull, Corey James, April Miller*

**Paper 372t:** Using Water to Engage Community College Students and Increase Graduation Rates — *Caryn L. Heldt, Christian Nwamba, Barbara Radecki*

**Paper 372u:** Assessing Preparedness of Transfer Students into Chemical Engineering in Comparison to Their Peers — *Amanda Simson, Elizabeth J. Biddinger*

**(373) Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange**

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Daniel W. Siderius, Chair  
Fateme Rezaei, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**Paper 373a:** The Separation of Sulfide in Polluted Air from Molecular Simulation — *Xumiao Zhou, Yuanyuan Yu, Li Yang*

**Paper 373b:** Continuous Li-Mining from Secondary Resources Via Electrospun Nanofiber Membrane Adsorber with Lithium Ion Sieves — *Rosemarie Ann I. Cuevas, Grace M. Nisola, Hiluf Tekle Fissaha, Erwin C. Escobar, Chosel P. Lawagon, Lawrence A. Limjoco, Rey Eliseo C. Torrejos, Seong-Poong Lee, Wook-Jin Chung*

**Paper 373c:** Preparation of Amine Modified Bimodal Mesoporous Silica Particles for CO<sub>2</sub> Separation — *Younghee Lee, Junichi Ida, Tatsushi Matsuyama*

**Paper 373d:** Ash Modified with Surface Active Agents for the Adsorption of Chloro/Nitro Benzenes from Aqueous Phase — *H M Zaheer Aslam, Sadiya Mushtaq*

**Paper 373e:** Synthesis of Zeolite X from Rice Husk Ash — *Hector D. Diaz Ortiz, Alvaro Orjuela, Jose H. Ramirez F., Gerardo Rodriguez, Hamid Godini, Erik Esche, Jens-Uwe Repke, Oliver Görke, Karla D. Guerrero G., Cristian C. Rodriguez*

**Paper 373f:** Synthesis and Adsorption Kinetics of Hierarchical 5A Zeolites — *Jichang Liu, Ruitong Wang, Congwei Zhong*

**Paper 373g:** Cr-, Fe-, and Ga-Doped CaO Adsorbents for High Temperature CO<sub>2</sub> Capture: An Adsorption and In-Situ XRD Study — *Ahmed Al-Mamoori, Ali Rowanaghi, Fateme Rezaei*



**(374) Poster Session: General Topics on Separations****Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Stephen Ritchie, Chair

Joshua A. Thompson, Co-Chair

**Sponsored by:** General Topics and Other Methods

**Paper 374a:** Development of Polymeric Ionic Liquid Thin Films for Ion-Selective Anion Exchange Membranes in Electrodialysis Separations — **Saloumeh Kolahchyan, Alexander M. Lopez**

**Paper 374b:** Zwitterionic Interactions with Charge Mosaic Membranes Prepared Via Electrohydrodynamic Jet Printing — **John R. Hoffman, William A. Phillip**

**Paper 374c:** Formation of Activated Carbon/Polymer Bilayer Membranes By Solution Electrospinning for Water Purification — **Jeremy Lewis, Keith M. Forward, Ali Alshami**

**Paper 374d:** The Synthesis of Thermally Rearranged Polyimide Membranes for Natural Gas Separation Using Four Different Dianhydride Precursors — **Maram Al-Sayaghi, Ali Alshami**

**Paper 374e:** Integrated Electrocoagulation-Ultrafiltration System for Treating Poultry Processing Wastewater — **Kamyar Sardari, Yu-Hsuan Chiao, S. Ranil Wickramasinghe**

**Paper 374f:** Determination of Binodal Curves and Tie Lines for Aqueous Two-Phase Systems with Osmolytes for Bioseparations — **Pratik U. Joshi, Seth Kriz, Michael Schroeder, Caryn L. Heldt**

**Paper 374g:** Understanding the Molecular Origin of Polymorphic Transition Mechanisms in Molecular Crystals — **Hyunjoong Chung, Ying Diao**

**(375) Poster Session: Particle Technology Forum****Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Manuk Colakyan, Co-Chair

Ray Cocco, Co-Chair

**Sponsored by:** Particle Technology Forum

**Paper 375a:** Direct Numerical Simulations of Hydrodynamic Forces on Assemblies of Non-Spherical Particles — **Sathish K.P. Sanjeevi, Johan T. Padding**

**Paper 375b:** Reactive Crystallization of Metal-Amino Acid Chelates and their Nucleation Kinetics — **Wang-Soo Kim, Chun-Il Park, Moonyong Lee, Young-Gyu Kim, Kee-Kahb Koo**

**Paper 375c:** Slurry Coating for Energetic Material Formulations — **Christopher Pizzo, Eric Gauthier**

**Paper 375d:** Investigation of Particle-Size Dependent Charging — **Xiaoyu Liu, Ifunanya Nwogbaga, Pranav Saba, Jari Kolehmainen, Ali Ozel, Troy Shinbrot, Sankaran Sundaresan**

**Paper 375e:** Effect of Particle Friction on Binary Granular Shear Flows of Inelastic Grains — **Jiecheng Yang, Yu Guo, Jennifer S. Curtis**

**Paper 375f:** Economic Analysis of Alternative Continuous Crystallization Technologies for Mass Production — **Kwan-Ling Wu, Jeffrey D. Ward**

**Paper 375g:** Bimetallic Atomic Layer Deposition for Extended Surface Electrocatalysts — **William McNeary IV, Annika Lai, Audrey Linico, Chilan Ngo, Sarah Zaccarine, Jason Zack, Katherine Hurst, Shaun M. Alia, Scott A. Mauger, K.C. Neyerlin, Karen J. Buechler, J. Will Medlin, Svitlana Pylypenko, Bryan S. Pivovar, Alan W. Weimer**

**Paper 375h:** An Experimental Study of Cylindrical Particle's Effective Size in a Rotating Tumbler — **Siying Liu, Joseph J. McCarthy**

**Paper 375i:** Laser Pyrolysis Synthesis of Novel Nanoparticles Using Spray-Based Precursor Delivery — **Mohammad Malekzadeh, Parham Rohani, Mayuresh Keskar, Mark T. Swihart**

**Paper 375j:** Particle Size Techniques/Capabilities Used in the Coatings Industry — **Chris Sierka, Kristin Nuzzio, Mike Werkmeister, Ethan Swope, Denise Schmidt**

**Paper 375k:** Modeling Granular Material Segregation Using a Multi-Scale Model — **Yu Liu, Marcial Gonzalez, Carl Wassgren**

**Paper 375l:** Oxidation of Fractal-like Soot Agglomerates — **Georgios A. Kelesidis, Sotiris E. Pratsinis**

**Paper 375m:** Experimentally Validated Computational Models to Predict the Impact of Humidity on the Flow of Pharmaceutical Mixtures — **Koyel Sen, Raj Mukherjee, Chen Mao, Bodhisattwa Chaudhuri**

**Paper 375n:** Conduction and Convection Heat Transfer in a Rotary Drum Using an Integrated PIV/IR Technique — **Manogna Adepu, Heather N. Emady**

**Paper 375o:** Light Alkane Valorization to Ethylene Via Chemical Looping Oxidative Dehydrogenation — **Vasudev Pralhad Haribal, Luke Neal, Seif Yusuf, Fanxing Li**

**Paper 375p:** Optimising Granulate Formulation through Uniaxial Powder Testing — **Tim Freeman, Jamie Clayton, John Yin, Rajeev Dattani**

**Paper 375q:** Optimising Powder Properties for DPI Capsule Filling Performance — **Tim Freeman, Rajeev Dattani, Jamie Clayton, John Yin, Dave Seaward, Jessica Binnie**

**Paper 375r:** The Effect of Storage Time on Flow Characteristics of Maic-Modified Compounds — **Charles R. Bowman, William A. Hendrickson, Tim Freeman, Christopher J. Rueb**

**Paper 375s:** Silicon Carbide and Carbon Double Shells Coated Silicon Nanoparticles for High Performance Lithium-Ion Batteries — **Chunhui Yu**

**Paper 375t:** Influence of Model Parameters on Runtime and Accuracy of CFD-DEM Simulations of a Prismatic Spouted Bed — **Thomas Eppinger, Leonard Becker, Felix Klippel, Oleh Baran, Ravindra Aglave**

**Paper 714b:** Bioinspired Silica: A Novel, Green and Biocompatible Drug Delivery System — **Scott Davidson, Dimitrios A. Lamprou, Andrew Urquhart, M. Helen Grant, Siddharth V. Patwardhan**

**Paper 375v:** Purdue University's Center for Particulate Products and Processes — **Dhananjay A. Pai, Carl Wassgren**

**Paper 375u:** A Roller Milling Simulator — **Grace Tshinguz Sr.**

**(376) Poster Session: Separations Division****Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Roger D. Whitley, Chair

Mark M. Davis, Co-Chair

**Sponsored by:** Separations Division**MEMBRANES**

**Paper 376a:** Imidazolium Based Poly(ionic liquids), the Tunable Membranes Having Antimicrobial Activity — **Arijit Sengupta, Sudhesh Kumar, Mohanad Kamaz, Mahmood Jebur, S. Ranil Wickramasinghe**

**Paper 376b:** Synthesis and Characterization of Novel Sulfonated Amine Block Copolymers for Direct Methanol Fuel Cells — **Karen Barrios-Tarazona, David Suleiman**

**Paper 376c:** Elucidating the Effects of Asymmetric Charge Patterning on Ion Transport through Charge Mosaic Membranes — **Feng Gao, William A. Phillip**

**Paper 376e:** Fundamental Pure and Mixed Liquid Sorption Properties of Osn Membranes Based on Polybenzimidazoles — **Tram Ngoc Pham, Kelly Bye, Judy Riffle, Michele Galizia**

**Paper 376f:** Ultra-Permeable Polyimide/MOFs Hybrid Membranes for Gas Separations — **Canghai Ma, Jeffrey J. Urban**

**Paper 376g:** Effects of Regiochemistry on the Properties and Gas Separation Performances of Ionic Polyimides — **Grayson P. Dennis, Kathryn E. O'Hara, Jason E. Bara**

**Paper 376h:** Improved Gas Separation Performance of Mixed-Linker Zeolitic Imidazolate Framework ZIF Membranes Via Post Synthetic Ligand Exchange — **Moon Joo Lee, Yu-Chen Hsu, Mohamad Rezi Abdul Hamid, Stephanie Bates, Hae-Kwon Jeong**

**Paper 376i:** Evaluation of Desorption and Diffusion in Zeolite Membrane with Nano-Perm Porometry — **Genki Kobayashi, Motomu Sakai, Masahiko Matsukata**

**Paper 376j:** Membrane Surface Modification Using Acrylate- and Thiol-Containing Zwitterionic Materials Via Polydopamine — **Nima Shahkaramipour, Chong Cheng, Haiqing Lin**

**Paper 376k:** Effect of Sulfonated Graphene Oxide Nanofiller on the Performance and Properties of Poly(vinyl alcohol) Thin Film Composite Forward Osmosis Membrane — **Anelyn Bendoy, Hana G. Zeweldi, Myoung Jun Park, Hanseung Kim, Wook-Jin Chung, Grace M. Nisola**



## ■ ADSORBENTS

**Paper 376bd:** Thermal Aging of Ag-MOR and Ag-Aerogel in Nuclear Off-Gas Streams Containing H<sub>2</sub>O and NO<sub>x</sub> — **Yue Nan, Seungrag Choi, Abney Carter, Jisue Moon, Jiuxu Liu, Lawrence L. Tavlirides**

**Paper 376be:** CO<sub>2</sub> Adsorption Performance of Functionalized Metal-Organic Frameworks with Different Topologies By Molecular Simulations — **Wei Li**

**Paper 376bf:** Fibrous Carbon Molecular Sieve with 3-5 Å Tunable Pores for Many Industrial Gas Separations (Poster) — **Jay (Junqiang) Liu, Janet Goss, Rob Golombeski, Ted Calverley**

**Paper 376bg:** Dependency of Shell Thickness of Smart Core-Shell Nanofibers for Water Capture and Release — **Soyoung Kim, Heechul Choi**

**Paper 376bh:** Selective Adsorbents Based on Thia-Crown Ether Functionalized Composite Mesoporous Silica for Selective Recovery of Silver Ions from Aqueous Sources — **Hiluf Tekle Fissaha, Grace M. Nisola, Lawrence A. Limjuco, Erwin C. Escobar, Wook-Jin Chung**

**Paper 376bi:** Study of Functional Groups of Ligands in Cu<sup>2+</sup> MOFs in the Efficiency and Selectivity of Gas Adsorption — **Rodrigo-Iván Dorantes-Martínez, Adriana-Itzel Cibrián-Juárez, Tomás-Eduardo Chávez-Miyauchi, Adriana Benítez-Rico**

**Paper 376bk:** Task-Specific Ionic Liquids Functionalized with Cobalt(II) Salen for Biomimetic Reversible Dioxigen Binding — **Qinghe Zheng, Marty Lail, Shaojun Zhou, Samuel Thompson, Kelly Amato**

**Paper 376bx:** Separation of Chitin from Shrimp Shells Using Functional Ionic Liquids — **Xingmei Lu**

## ■ CRYSTALLIZATION

**Paper 376bl:** Separation of Ammonium Iodide and 1,4-Phenylenediamine from Their Mixture — **Jae-Kyeong Kim, Hyun-Joo Lee, Wang-Soo Kim, Yong-Ki Park, Kee-Kahb Koo**

**Paper 376bm:** Amorphization of Azilsartan By Drowning-out Crystallization Combined with Freeze-Drying — **Chun-Il Park, Su-Kwang Kim, Kee-Kahb Koo**

**Paper 376bn:** Purification of L-Menthyl Enantiomers from the Racemic Mixture By Stripping Crystallization — **Lie-Ding Shiau**

## ■ PROCESSES

**Paper 376bo:** Continuous High-Purity Recovery of Xylobiose from the Output of *Bacillus Pumilus*  $\beta$ -Xylosidase Reaction Using a Well-Designed Simulated Moving Bed Process — **Hangil Park, Jae-Hwan Choi, Chanhun Park, Sungyong Mun**

**Paper 376bp:** Effect of Rotating Elements on HETP of a Horizontal Distillation Column — **Yusuke Shimada, Yumi Uno, Ken-Ichiro Sotowa, Toshihide Horikawa, Jesus Rafael Alcantara-Avila**

**Paper 376bq:** Numerical Investigation of the Effect of Bend on the Gas Absorption Rate in Microchannels — **Takumi Nishimoto, Ken-Ichiro Sotowa, Toshihide Horikawa, Jesus Rafael Alcantara-Avila**

**Paper 376br:** Methyl Palmitate Separation from the Reaction Mixture of the Solvent-Free Transesterification to Produce Sucrose Esters — **Javier Chavarrio, Maria F. Gutierrez, Alvaro Orjuela**

**Paper 376bs:** Ultrasound-Mediated Nonequilibrium Separation of Ethanol-Water Solutions, Including Avoidance of the Azeotropic Bottleneck — **Ozan Kahraman, Arne Pearlstein, Hao Feng**

**Paper 376bt:** Techno-Economic Analysis of Deep Eutectic Solvent Based SO<sub>2</sub>-CO<sub>2</sub> Co-Capture Process for Flue Gas — **Kyle McGaughey, M. Toufik Reza**

**Paper 376bu:** Optimization of Distillation Processes — **Reza Haghpannah, Greg Theunick**

**Paper 376bv:** Multi-Objective Optimization of a Batch Distillation Column — **Sidharth Sankar Parhi, Gade Pandu Rangaiah, Amiya Kumar Jana**

**Paper 376bw:** A Novel FO-MED Hybrid System for MED Brine Further Concentration — **Ye Yang, Yuzhu Sun, Jianguo Yu**

**Paper 438a:** Predicting the Productivity of Chromatography Processes By Repeated Cyclic Operations or By Continuous Column Switching Operations — **Noriko Yoshimoto, Shuichi Yamamoto**

## (377) Poster Session: Thermodynamics and Transport Properties (Area 1A)

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Andrew Paluch, Chair

**Sponsored by:** Thermodynamics and Transport Properties

## ■ PROPERTY PREDICTION AND CORRELATION

**Paper 377a:** Prediction of Critical Properties and Vapor Pressure from PR+Cosmosac Eos Based on Different Quantum Mechanical Calculations — **Hsing-Hao Liang, Chieh-Ming Hsieh**

**Paper 377b:** Modeling of Excess Molar Volumes for Binary Mixtures Containing (Dimethyl Carbonate (DMC) + Alcohol) at  $T = (288.15 - 308.15)$  K and Atmospheric Pressure — **Gustavo V. Olivieri, Ricardo B. Torres**

**Paper 377c:** Modeling of Excess Molar Volumes for Binary Mixtures Containing {2-(dimethylamino)Ethyl Methacrylate + Alcohol} at  $T = (293.15 - 313.15)$  K and Atmospheric Pressure — **Dereck N. F. Muche, Gustavo V. Olivieri, Ricardo B. Torres**

**Paper 377d:** Correlation of Kinematic Viscosities for CO<sub>2</sub> + Co-Solvent Systems at High Pressures By Modified Eyring and Wilson-Visco Method — **Katsumi Tochigi, Hiroyuki Matsuda, Kiyofumi Kurihara, Toshitaka Funazukuri, V.K. Rattan**

**Paper 377e:** Molecular Thermodynamic Modelling of Micellar-Assisted Drug Delivery Systems — **Arthur S. Gow, Thomas Hong**

**Paper 377f:** Modeling the Optical Properties of Silica Aerogel — **Hannah Margavio, Sungwoo Yang**

**Paper 377g:** Study of Isothermal Solubilities of Benzene, DCE, DCM, and Chloroform in Diblock and Triblock Copolymers of Polycaprolactone and Polyethylene Glycol at 298.15K Using a QCM — **Abhijeet Iyer, Scott W. Campbell, Venkat R. Bhethanabotla**

**Paper 377h:** Reaction Models Describing Antioxidant Depletion in Polyethylene, Polypropylene and Polyvinyl-Chloride Caused By Thermal Degradation — **Iftekhar Ahmad, Mohammed Faizan Khoker, Mohammad Sarafraj**

**Paper 377i:** Modeling Olanzapine Solution Growth Morphologies — **Yuanyuan Sun, Carl Tilbury, Susan M. Reutzel-Edens, Jinjin Li, Michael F. Doherty**

**Paper 377j:** Mechanism of SO<sub>2</sub> absorption in Ionic Liquids — **Xiaochun Zhang, Suojang Zhang, Shaojuan Zeng**

## ■ MOLECULAR SIMULATION

**Paper 377j:** Bridging Two-Liquid Theory with Molecular Simulations for Electrolytes: An Investigation of Aqueous NaCl Solution — **Sina Hassanjani Saravi, Ashwin Ravichandran, Rajesh Khare, Chau-Chyun Chen**

**Paper 377k:** Molecular Simulation on Human Beta Defensin Type 3 Interaction with Lipid Membranes — **Liqun Zhang, Christopher Elson**

**Paper 377l:** Theoretical Detection of a HDA-Lda Liquid-Liquid Transition Phase for Water Using Molecular Simulation — **Rafael Risnik Romeiro, Pedro A Pessoa Filho**

## ■ PHASE EQUILIBRIUM MEASUREMENTS

**Paper 377m:** Volumetric, Acoustic and Viscometric Properties of Binary Mixture of (*n*-butylammonium methanoate + 1-butanol) at Different Temperatures — **Robert L. Fernandes, Heloisa E. Hoga, Ricardo B. Torres**

**Paper 377n:** Measurements and Calculations of Asphaltene Deposition — **Adel Elsharkawy, Maryam Al-Matrouk**

**Paper 377o:** Sorption of Benzene, Toluene, Ethyl Benzene and Xylene By Polymer/Plasticizer Blends Using Quartz Crystal Microbalance — **Kiranpreet Kaur, Abhijeet Iyer, Scott W. Campbell, Venkat R. Bhethanabotla**

**Paper 377p:** Volumetric and Spectroscopic Properties of Binary Mixtures of {Diethyl Malonate + Acetonitrile} at Different Temperatures and Atmospheric Pressure — **P. J. Castro, Heloisa E. Hoga, Ricardo B. Torres**

**Paper 377q:** Rapid Methane Hydrate Formation with Cyclopentane Hydrate Seed Crystals — **Seungjun Baek, Yun-Ho Ahn, Junshe Zhang, Juwon Min, Wonhyeong Lee, Jae W. Lee**

## ■ QUANTUM CHEMISTRY

**Paper 377r:** Predictions of Gas Phase Thermochemical Properties from Ab Initio Calculation: Applications to Bio-Oil Compounds — **Detlev C. Mielczarek, Patrice Paricaud, Chourouk Nait Saidi, Laurent Catoire**

**Paper 377t:** Simulation and Thermodynamic Performance Evaluation of a Flash Tank Vapor Injection Refrigeration System Using Mixed Refrigerants — *Giulia L.M. Trazzi, José Vicente H. D'Angelo, Ricardo B. Torres*

### (378) Poster Session: Transport and Energy Processes

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Exhibit Hall B

Haider Al-Rubaye, Chair

**Sponsored by:** Transport and Energy Processes

**Paper 378a:** Effect of Shear Rate and Drying Speed in Lithium Ion Battery Slurry Processing — *Renee Saraka, Samantha Morelly, Maureen H. Tang, Nicolas J. Alvarez*

**Paper 378b:** Improving Electrode Performances for Air-Cathode Microbial Fuel Cells — *Yu-Chieh Huang, Shi-Chern Yen*

**Paper 378c:** Solar Hybrid Power Systems for Improved Electrical Delivery in Low Humidity, High Temperature Conditions — *Mounir Bouzguenda, Aly A Aboulhaga, Gafar Elamin, Kenneth L. Roberts*

**Paper 378d:** Lithium Iron Phosphate-Graphene Composite Cathode Materials for Lithium Ion Battery with Improved Rate Capability — *Manik Biswas, Ju-Won Jeon*

**Paper 378e:** Comparative Study of Graphene/Water Nano-Fluid in a Heat Exchanger System: Modelling and Simulation — *Akshya Khandelwal, Devendra Purbia, Arvind Kumar Sharma*

**Paper 378f:** Electrochemical Studies of Low Temperature Ionic Liquid-Cosolvent-Salt Electrolyte Systems — *Wendy J. Lin, Yifei Xu, Marisa E. Gliege, Zuofeng Zhao, Hongyu Yu, Lenore L. Dai*

**Paper 378g:** Stability of Oil-in-Water Emulsions of Heavy Crude Under Flowing Conditions — *Yue Cui, Qiyu Huang, Jiadi Zhao, Weidong Li, Caoding Wang*

**Paper 378h:** Thermal Distribution on a Heating FLAT Plated Cooled with a Swirling Impinging Jet — *Smith Eiamsa-ard, K. Kunarak, K. Wongcharee, V. Chuwattanakul*

**Paper 378i:** Periodically FULLY Developed Laminar FLOW and HEAT Transfer Characteristics in Tubes Inserted with Rectangular-CUT Twisted Tapes — *V. Kongkaitpaiboon, A. Sroysri, K. Wongcharee, V. Chuwattanakul, M. Pimsarn, Smith Eiamsa-ard*

**Paper 378j:** Concept to Commercialization: Energy efficient & Eco-friendly Anode Grade Coker Technology — *Satyen Kumar Das, T.H.V.D. Prasad, Pradeep P.R., Madhusudan Sau, Debasis Bhattacharyya, S.K. Majumdar, S. S. V. Ramakumar*

**Paper 378k:** Quantified Investigation of Coal Ash Fusion Behavior for Gasifier Design and Operation — *Jin Bai, Lingxue Kong, Xiaoming Li*

**Paper 378l:** Molecular Insight into the Growth of Hydrogen and Methane Binary Hydrates — *Zhengcai Zhang*

**Paper 378m:** Conversion from CO<sub>2</sub>-Containing Flue Gas to Electrocatalysts — *Seoyeon Baik, Bong Lim Suh, Ayeong Byeon, Jihan Kim, Jae W. Lee*

**Paper 378n:** Composite Electrolytes of Pyrrolidone-Derivatives-PEO Enable to Enhance Performance of All Solid State Lithium-Ion Batteries — *Xin Li, Yidong Liu, Yong Min*

**Paper 378o:** The Effect of Micro and Nano Material on Critical Heat Flux (CHF) Enhancement — *Jamal Al-Rubaye, Enas Sheref*

**Paper 378q:** Direct Power Generation from Reed Biochar in a Direct Carbon Fuel Cell — *Jun Wang, Yongdan Li*

**Paper 378r:** A LaNi<sub>0.9</sub>Co<sub>0.1</sub>O<sub>3</sub> Coated Ce<sub>0.8</sub>Sm<sub>0.2</sub>O<sub>1.9</sub> Composite Anode for Solid Oxide Fuel Cells Fed with Methanol — *Tian Gan, Yongdan Li*

**Paper 378s:** Effect of Geometry, Gas Flow Rates, and Oxygen Concentration on the Performance of Anode-Supported Planar SOFCs — *Nayan Biswas, Deepra Bhattacharya, Jayanta Mukhopadhyay, Rajendra Nath Basu, Prasanta Kumar Das*

**Paper 378t:** Experimental Optimization of Design Parameters of Cylindrical PEM Fuel Cell and Diagnosis of Its Performance Degradation — *Suseendiran S. Ravichandran, Samuel Pearn-Rowe, Raghunathan Rengaswamy*

**Paper 378u:** Organic Rankine Cycle Waste Heat Recovery System to Cool the Data Center — *M. Toufiq Reza, Russ Tipton*

**Paper 378v:** Energy Optimization By Installation of Heat Recovery Steam Generator at Exhaust Gases of Gas Turbine Driven Compressor (Engro Fertilizers Limited) — *Kashif Jameel, Sannan Aleem, Bilal Mustafa*

**Paper 378w:** Understanding the Single Pass Operation of Vrbf and the Associated Mass Transfer Loss — *Deepa Elizabeth Eapen, Raghunathan Rengaswamy*

**Paper 378x:** CZTS (Cu<sub>2</sub>ZnSnS<sub>4</sub>) Electrode for Solar Rechargeable Polysulfide Bromide Redox Flow Battery — *Animesh Mondal, James G. Radich*

**Paper 378y:** Cuprous Bromide: An Examination of High Halide Copper Electrodeposition and Its Application in a Flow Battery — *Elizabeth A. Stricker, Jesse S. Wainright, Robert F. Savinell*

**Paper 378z:** A Low-Dimensional Electrochemical Model for Scaling and System Analysis of Redox Flow Batteries — *John L. Barton, Fikile Brushett*

**Paper 378aa:** Highly Selective Electroreduction of Carbon Dioxide into Fuels with High Current Density on Mesoporous Copper Oxide-Derived Inverse Opals — *Thuy-Duong Nguyen-Phan, Douglas R. Kauffman, Yang Yu, Yunyun Zhou, Bret H. Howard, Mengling Y. Stuckman, Paul R. Ohodnicki*

**Paper 378ab:** Enhancing the Stability of High-Voltage Lithium-Ion Battery Using Sulfur-Containing Electrolyte Additives — *Xiaoying Yu II, Chao Shang, Qi Wang*

**Paper 378ac:** A Molecular Simulation Study for Natural Gas Upgrading through Mixed-Matrix Membranes Formed By PB-1A Organic Cage and a Polymer with Intrinsic Microporosity — *Zeyu Zhao, Jie Liu, Jianwen Jiang*

**Paper 378ad:** The Effect of Aluminum Short-Range Ordering on Carbon Dioxide Adsorption in Zeolites — *John Findley*

**Paper 378ae:** Computational Screening of Hydration Reactions for Thermal Energy Storage: New Materials and Design Rules — *Steven Kiyabu, Jeffrey S. Lowe, Alauddin Ahmed, Donald J. Siegel*

**Paper 378af:** A Combined Adsorbent Bed and Pellet Model for Adsorptive Hydrogen Storage — *Palla Sridhar, Niket S. Kaisare*

**Paper 378ag:** High Energy Density Energy Storage System Composed of Electrolyzer, Metal Hydride, and Fuel Cell — *Gwangwoo Han, Joongbae Kim, Yongkeun Kwon, Sungbaek Cho, Joongmyeon Bae*

**Paper 378ah:** Heat and Mass Transfer of Complex Metal Hydride Hydrogen Storage Reactor with Improved Heat Exchange System: Modelling and Simulation — *Sibusiso E. Mavuso, Thabang Ntho, Andrei V. Kolesnikov*

**Paper 378ai:** A Symmetrical Solid Oxide Fuel Cell with a-Site Sodium Doped Perovskite Electrode Materials — *Tongtong Yao, Yongdan Li*

**Paper 378ak:** Humidity Tracking By Mixing Dry and Humidified Gases with Internal Model Control for PEM Fuel Cells — *Sathish Swaminathan, Srinivasan Raman, Raghunathan Rengaswamy*

**Paper 378al:** A Macroscopic Model Accounting for the Composite Effects for an Ion Lithium Cell with a LiFePO<sub>4</sub> Cathode — *Ilda Santos, Ignacio Gonzalez, Jorge Vazquez-Arenas, Carlos Omar Castillo-Araiza*

**Paper 378am:** Research of the Vertical Falling Film Behavior in the Scrubbing-Cooling Tube — *Yifei Wang, Xin Peng, Liucheng Yan, Guangsu Yu, Fuchen Wang*

### (379) Active Colloidal Systems

**Tuesday, Oct 30, 3:30 PM**

Omni William Penn Hotel, Conference Center B

Bhuvnesh Bharti, Chair

Christopher L. Wirth, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 379a:** Reconfigurable Paramagnetic Colloidal Microswimmers Using Time-Varying Magnetic Fields — *Sibani Lisa Biswal*

**3:45 Paper 379b:** Aggregation and Fragmentation of Active Superparamagnetic Colloidal Chains — *Ronal A. DeLaCruz-Araujo, Luis Y. Rivera-Rivera, Ubaldo M. Córdoba-Figueroa*

**4:00 Paper 379c:** Directed Motion and Programmed Assembly of Actively Rotating Colloids — *Jin Gyun Lee, Bhuvnesh Bharti*

**4:15 Paper 379d:** Directional Migration of Active and Inactive Liposomes — *Ambika Somasundar, Farzad Mohajerani, Subhadip Ghosh, Darrell Velegol, Ayusman Sen*

**4:30 Paper 379e:** Magnetic Janus Particle Chain Length's Influence on Assembly Rate — **Thomas Long, Ilona Kretzschmar**

**4:45 Paper 379f:** Tailoring Active Matter Collective Behavior through Particle Anisotropy — **Shannon E. Moran, Isaac R. Bruss, Sharon C. Glotzer**

**5:00 Paper 379g:** Programming Shape and Motion into Active Loops — **Mayank Agrawal, Sharon C. Glotzer**

**5:15 Paper 379h:** Active Motion of Liquid Crystal-in-Liquid Crystal Emulsions — **Karthik Nayani, Nicholas L. Abbott**

**5:30 Paper 379i:** Shape-Directed Motion of Homogeneous Catalytic Micromotors — **Allan M. Brooks, Mykola Tasinkevych, Syeda Sabrina, Darrell Velegol, Kyle J. M. Bishop, Ayusman Sen**

**5:45 Paper 379j:** Engineering Phase Transitions of Colloidal Crystals By Inverse Design — **Chrisy Xiyu Du, Greg van Anders, Julia Dshemuchadse, Paul Dodd, Sharon C. Glotzer**

### **(380) Advanced Nanomaterial Catalysts for Clean, Sustainable Technologies**

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 403

Yang Zheng, Chair  
Homa Khosravian, Co-Chair  
Praveen Bollini, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 380a:** Towards Rational Synthesis and Molecular Level Understanding of Pd/Zeolite Passive NO<sub>x</sub> Adsorber (PNA) Materials — **Konstantin Khivantsev, Nicholas Jaegers, Libor Kovarik, Yanran Cui, Franklin (Feng) Tao, Jonathan C. Hanson, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Yong Wang, Feng Gao, Janos Szanyi**

**3:48 Paper 380b:** Sulfur Dioxide Oxidation Studies with Precious Metal Catalysts: Sulfur Surface Species Stability Versus Adsorption Amount Impact on Activity Loss — **Monique Shauntá Wilburn, William S. Epling**

**4:06 Paper 380c:** Kinetic Study of the Reduction and Oxidation Half-Cycles during Selective Catalytic Reduction of NO<sub>x</sub> with Ammonia on Cu-SSZ-13 — **Ishant Khurana, Arthur J. Shih, Sichi Li, Casey Jones, Aleksey Yezerets, W.N. Delgass, Jeffrey T. Miller, William F. Schneider, Rajamani Gounder, Fabio H. Ribeiro**

**4:24 Paper 380d:** Pd@CeO<sub>2</sub> Core@Shell Nanoparticles: Enhancing Thermal Stability and Activity in Three-Way Automotive Catalysts — **Alexander Hill, Chang Yup Seo, Johannes W. Schwank, Andrej Lenert**

**4:42 Paper 380e:** Multi-Scale Modelling of Gasoline Particulate Filters – How the Porous Structure of Filter Affects Its Performance — **Marek Vaclavik, Marie Placha, Martin Isoz, Martin Leskovjan, Panagiotis Boutikos, Petr Koci, Milos Svoboda, Emily Price, Vladimir Novak, David Thompsett**

**5:00 Paper 380f:** Assessing the Catalytic Applicability of Zirconium and Cerium Oxide Microspheres Prepared By Internal Gelation — **Jae-Soon Choi, Jack L. Collins, Ercan Cakmak, Michael J. Lance, Rodney D. Hunt**

**5:18 Paper 380g:** Tuning ZSM-11 Catalyst Performance in the Methanol-to-Hydrocarbon Reaction through Controlled Post-Synthesis Modification — **Thuy T. Le, Heng Dai, Jeffrey D. Rimer**

### **(381) Advancements in Particle Engineering for Crystallization in Pharmaceutical Process Development**

**Tuesday, Oct 30, 3:30 PM**  
Westin Convention Center, Fayette

Lei Zhu, Chair  
Samir Kulkarni, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 381a:** Crystal Engineering of Needle Shaped API - a Mechanistic Modelling Approach — **Anna Jawor-Baczynska, Leonor Rosa, Niall Mitchell**

**3:50 Paper 381b:** Strategies for Crystallization Development of Process Intermediates in Early and Late Stage Manufacturing Processes — **David W. Place**

**4:10 Paper 381c:** Polymorphism Control Via Combined Cooling and Antisolvent Crystallization in Continuous Mixed Suspension Mixed Product Removal Crystallizers — **Shivani Kshirsagar, Botond Szilagyi, Zoltan K. Nagy**

**4:35 Paper 381d:** Anticipate and Avoid Oiling out in Crystallization Using Molecular Dynamics Simulations — **Deepak Jain, Joydeep Kant, Vishwanath Dalvi, Channamallikarjun Mathpati**

**4:55 Paper 381e:** Controlling Crystal Size Via Fine Particle Dissolution in a Closed Loop Wet Milling Crystallization — **Kirankumar Ramisetty, Ake Rasmuson, Tom O'Ceallaigh, Aaron Cote, Denise Croker**

**5:20 Paper 381f:** Sonoseeding: An Alternative Approach for Scale-up of Batch Sonocrystallization — **Kirankumar Ramisetty, Vasanth Kumar Kannuchamy, Ake Rasmuson**

**5:45 Paper 381g:** Crystal Form and Morphology Control of Obeticholic Acid by Crystallization in Selected Solvents — **Shichao Du, Yan Wang, Junbo Gong, Xiaoyue Tan**

### **(382) Advances in Process Control II**

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 408

Nael H. El-Farra, Chair  
Victor M. Zavala, Co-Chair

**Sponsored by:** Systems and Process Control

**3:30 Paper 382a:** On Integration of Feedback Control and Safety Systems: Studying a High-Pressure Flash Drum Separator — **Zhihao Zhang, Zhe Wu, Helen Durand, Panagiotis D. Christofides**

**3:49 Paper 382b:** Two Feedback Control Schemes for the Size and Shape of Needle-like Crystals Growing in Suspension — **Stefan Boetschi, Ashwin Kumar Rajagopalan, Manfred Morari, Marco Mazzotti**

**4:08 Paper 382c:** Robust Fault Tolerant Control of Hydraulic Pipeline Systems — **Xiaodong Xu, Stevan Djuljevic**

**4:27 Paper 382d:** Learning-Based Nonlinear Model Predictive Control with Chance Constraints for Stochastic Systems — **Angelo D. Bonzanini, Tito Santos, Ali Mesbah**

**4:46 Paper 382e:** Control Under Uncertainty in Automated Drug Delivery — **Mudassir Rashid, Iman Hajizadeh, Ali Cinar**

**5:05 Paper 382f:** Predictive Control with Model Performance Monitoring and Re-Identification — **Masoud Kheradmandi, Prashant Mhaskar**

**5:24 Paper 382g:** Advanced Biomimetic Control Approach Integrated with Multi-Agent Optimization for Nonlinear Chemical Processes — **Gaurav Mirlekar, Berhane Gebreslassie, Urmila M. Diwekar, Fernando V. Lima**

**5:43 Paper 382h:** Nonlinear Optimal Control Structure Design — **Temitayo Bankole, Debansu Bhattacharyya**

### **(383) AIChE Journal Futures: New Directions in Chemical Engineering Research (Invited Talks)**

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 304

Michael Harold, Chair  
Prodromos Daoutidis, Co-Chair

**Sponsored by:** Publication Committee

**3:30** Introductory Remarks

**3:36 Paper 383a:** Rheological Properties and Structure of Step- and Chain-Growth Gels Concentrated above the Overlap Concentration — **Kelly M. Schultz**

**3:59 Paper 383b:** Dynamic Optimization with Pseudo-Transient Models: Theory and Application to PSA and Simulated Moving Bed Chromatography — **Michael Baldea**

**4:22 Paper 383c:** Stem Cell Biomanufacturing under Uncertainty: A Case Study in Optimizing Red Blood Cell Production — **Ruth Misener**

**4:45 Paper 383d:** Recombinantly Expressed Gas Vesicles as Nanoscale Contrast Agents for Ultrasound and Hyperpolarized MRI — **Mikhail G. Shapiro**

**5:08 Paper 383e:** Microfluidic Synthesis of Elastomeric Microparticles: A Case Study in Catalysis of Palladium-Mediated Cross-Coupling — **Milad Abolhasani**

**5:31 Paper 383f:** Effect of Peptide Linker Length and Composition on Immobilization and Catalysis of Leucine Zipper-Enzyme Fusion Proteins — **Julie A. Champion**

**5:54** Concluding Remarks

### **(384) AIChE's 110 Year Celebration (Invited Talks)**

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 303

Lorenz T. Biegler, Chair  
J. Karl Johnson, Co-Chair  
Cliff Kowall, Co-Chair

**Sponsored by:** Miscellaneous

**3:30** Welcoming Remarks

**3:35 Paper 384a:** 25 by 25: Chemical Engineering in the Next 25 Years — **Clare McCabe, Phillip R. Westmoreland**



**4:03 Paper 384b:** The Future of Chemical Engineering Itself — *Phillip R. Westmoreland*

**4:31 Paper 384e:** Accelerating Innovation through Academic-Industrial Partnerships — *William Liechty, Shawn D. Feist*

**4:59 Paper 384c:** Maximizing Uptime, Efficiency, and Safety of Industrial Operations through Early Risk Detection — *Ankur Pariyani*

**5:27 Paper 384d:** Gaussian Processes for Hybridizing Analytical & Data-Driven Decision-Making — *Simon Olofsson, Johannes Wiebe, Marc Peter Deisenroth, Ruth Misener*

**5:55** Concluding Remarks

### (385) Applied Project Management Fundamentals: A Tutorial

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 331

Eldon Larsen, Chair

**Sponsored by:** Management Division

**3:30 Paper 385a:** Introduction to the Fundamentals of Project Management — *Eldon Larsen*

**3:55 Paper 385b:** The Importance of People in Project Management — *Eldon Larsen*

**4:20 Paper 385c:** Communication--a Better Understanding — *Eldon Larsen*

**4:45 Paper 385d:** Planning and Conducting Effective Meetings — *Eldon Larsen*

**5:10 Paper 385e:** The Importance of Excellent Definition of Project Objectives — *Eldon Larsen*

**5:35 Paper 385f:** Overview of Project Planning — *Eldon Larsen*

### (386) Biomaterials: Graduate Student Award Session

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 328

Gulden Camci-Unal, Co-Chair  
Kyle Lampe, Co-Chair

**Sponsored by:** Biomaterials

**3:30 Paper 386a:** "Graduate Student Award Session:" Force-Responsive, Cryptic Hydrogels to Sense and Respond to Cell Traction — *Yen Tran, Matthew Rasmuson, Todd Emrick, John Klier, Shelly Peyton*

**3:44 Paper 386b:** Graduate Student Award Session: *In Vivo* Characterization of Glucose Responsive Insulin Delivery Systems — *Lisa R. Volpatti, Morgan Matranga, Abel B. Cortinas, Robert Langer, Daniel G. Anderson*

**3:58 Paper 386c:** Graduate Student Award Session: Enhanced Capture and Release of Circulating Tumor Cells Using Hollow Glass Microspheres with Nanostructured Surface — *Ziye Dong, Dan Yu, Wei Li*

**4:12 Paper 386d:** Graduate Student Award Session: Engineering Co-Culture of Cultured Glioblastoma Cells and Astrocytes to Study Cell-Cell Communication in GBM — *Kimberly M Stanke, Christina Wilson, Erin Eickman, Oleh Khalimonchuk, Srivatsan Kidambi*

**4:26 Paper 386e:** Graduate Student Award Session: Incorporating Electrospun Fiber Topography in a 3D PEG Hydrogel Promotes Oligodendrocyte Maturation — *Lauren Russell, Ethan Purnell, Kyle Lampe*

**4:40 Paper 386f:** Graduate Student Award Session: Tissue Guided Design of a Brain ECM Mimicking Hydrogel — *Sualyneth Galarza, Shelly Peyton*

**4:54 Paper 386g:** Graduate Student Award Session: A Three-Dimensional Hyaluronic Acid Hydrogel Platform to Study the Mechanobiology and Invasion of Brain Metastatic Breast Cancer Cells — *Akshay Narkhede, James Crenshaw, Riley Manning, Shreyas Rao*

**5:08 Paper 386h:** Graduate Student Award Session: Physically Crosslinked DNA-Based Injectable Hydrogels for Bone Regeneration — *Sayantani Basu, Settimo Pacelli, Arghya Paul*

**5:22 Paper 386i:** Graduate Student Award Session: Silica Nanoparticles Enable Oral Delivery of Insulin — *Nicholas G. Lamson, Adrian Berger, Kathryn A. Whitehead*

**5:36 Paper 386j:** Graduate Student Award Session: Application of Hydrogen Sulfide Releasing Materials in Complex Bone Regeneration — *Soheila Aliakbarighavimi, Ethan Lungren, Trent Faulkner, Brittany Allen, Jessica Stromsdorfer, Ram Rao Tata, Bret Ulrey*

### (387) Bionanotechnology Graduate Student Award Session

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 310

Lorraine Leon, Chair  
Millicent O. Sullivan, Co-Chair  
Kathryn A. Whitehead, Co-Chair

**Sponsored by:** Bionanotechnology

**3:30 Paper 387a:** Award Submission: Overcome Drug Resistance of Cancer Cells By Confining, Perturbing and Analyzing Them in Nano-Liter Chambers One Cell at a Time — *Yapeng Su, Wei Wei, Lidia Robert, Min Xue, Antoni Ribas, James Heath*

**3:50 Paper 387b:** Award Submission: Chitosan / Cellulose Nanocrystals / Calcium Phosphate Hydrogels for Vertebral Compression Fracture Treatment — *Soheila Aliakbarighavimi, Ethan Lungren, Josselet Allison, Yisheng Sun, Trent Faulkner, Ferris Pfeiffer, Christina Goldstein, Caixia Wan, Bret Ulrey*

**4:10 Paper 387c:** Award Submission: The Binary Effect on Drug-Resistant Bacteria of Polymeric Vesicles Appended By Proline-Rich Amino Acid Sequences and Inorganic Nanoparticles — *Nicole Bassous, Thomas J. Webster*

**4:30 Paper 387d:** Award Submission: Lipid Nanoparticle Ionization at Endosomal pH Is a Cell-Free Predictor of mRNA Delivery Efficacy In Vivo — *Khalid A. Hajj, Rebecca Ball, Sarah Deluty, Shridhar Singh, Christopher Knapp, Kathryn A. Whitehead*

**4:50 Paper 387e:** Award Submission: Nanomagnetic Illuminators for In Vivo Optical Imaging of Osteoarthritic Knee Joints — *Mythreyi Unni, Brittany Partain, Kyle Allen, Carlos Rinaldi*

**5:10 Paper 387f:** Award Submission: Quantification of Inflammatory Response and Morphological Change of SIM-A9 Microglia By Neuro-Probes — *Darwin Yang, Markita Landry*

**5:30 Paper 387g:** Award Submission: Cardiac Troponin I Detection Using Antibody-Immobilized Disposable Cover Glass and AlGaIn/GaN High Electron Mobility Transistors — *Jiancheng Yang, Patrick Carey IV, Fan Ren, Yu-lin Wang, Michael L. Good, Soohwang Jang, Michael A. Mastro, Stephen J Pearton*

### (388) Biosensor Devices: Applications II

**Tuesday, Oct 30, 3:30 PM**  
Westin Convention Center, Pennsylvania West

Qingshan Wei, Chair  
Kevin J. Cash, Co-Chair

**Sponsored by:** Sensors

**3:30 Paper 388a:** Invited Talk: The Next Dimension of Detection: Biomechanical Analysis of Tissue — *Andrea M. Armani, Alexa Hudnut, Lili Lash-Rosenberg, An Xin, Juan Doblado, Cecilia Zurita-Lopez, Qiming Wang*

**4:00 Paper 388b:** Rapid Biosensing of Endocrine Disruptors with Cell-Free Protein Synthesis — *Bradley C. Bundy, J Porter Hunt, Seung Ook Yang, Miriam Shakalli Tang, David W. Wood*

**4:20 Paper 388c:** Lab-on-Skin: Epidermal Microfluidic Device for the Capture, Storage, and Colorimetric Sensing of Sweat — *Yi Zhang, John A. Rogers*

**4:40 Paper 388d:** Stimulus Response Characterization of an Elastin-like-Polymer Modified Surface for Biosensor Applications — *Marissa Morales, Eva Rose M. Balog, Jeffrey M. Halpern*

**5:00 Paper 388e:** Development of a Unique Dual Ionophore Ion Selective Electrode for the Detection of Proteins and Cells — *Olivia Reynolds, Xuesong Li, Bernard J. Van Wie*

**5:20 Paper 388f:** Evaluation of Aptamer Technology for Detection of Quorum Sensing Molecules Produced By *Pseudomonas Aeruginosa* — *Pranali Buch, Edgar D. Goluch*

**5:40 Paper 388g:** Chromogenic Ethanol Sensors Enabled By Multi-Stimuli-Responsive Shape Memory Polymers — *Abdullateef Gari, Peng Jiang*

### (389) Computational Catalysis III: Electrocatalysis

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 402

Ronald Michalsky, Chair  
Craig Plaisance, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 389a:** Understanding the Importance of High Coverages in Electro-Catalysed Reduction of NO on Pt-Sn Alloys — *Siddharth Deshpande, Jeffrey Greeley*



**3:48 Paper 389b:** Probing the Intrinsic Reaction Barriers of HER in Acidic and Alkaline Media Using Electronic Structure Theory — **Per Lindgren**, Georg Kastlunger, Andrew A. Peterson

**4:06 Paper 389c:** First-Principles Prediction of Activated Carbon Nanostructures for Catalyzing Oxygen Reduction — **Gregory Hartmann**, Gyeong S. Hwang

**4:24 Paper 389d:** Quantifying Confidence in DFT Predicted Surface Pourbaix Diagrams and Associated Reaction Pathways for Chlorine Evolution — **Vaidish Sumaria**, Dilip Krishnamurthy, Venkatasubramanian Viswanathan

**4:42 Paper 389e:** A Roadmap for Modeling Single-Site (electro)Catalysts: A Combined Coupled Cluster, DFT and a Classical Force Field Approach — **Jens Nørskov**, Anjali M. Patel, **Ambarish Kulkarni**

**5:00 Paper 389f:** The Effect of Electrode Potential on the Stability of Intermediates Involved in Both Electrochemical CO<sub>2</sub> Reduction and Hydrogen Evolution — **Haochen Zhang**, William A. Goddard III, Qi Lu, Mu-Jeng Cheng

**5:18 Paper 389g:** Trends in Electrochemical Oxygen Reduction and Evolution Activities of Layered Double Hydroxides — **Zhenghang Zhao**, Ambarish R. Kulkarni, Michal Bajdich, Jens Nørskov

### (390) Conceptual Process Design in Refining, Petrochemicals and Gas Processing

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 323

Shu Wang, Chair  
Jia Li, Co-Chair

**Sponsored by:** Fuels and Petrochemicals Division

**3:30 Paper 390a:** A Multi-Objective Multi-Technology (MOMT) Framework to Evaluate Various Ammonia Synthesis Processes — **Jia Li**

**3:48 Paper 390b:** Process Simulation and Energy Analysis of Carbon Dioxide Removal in the Ammonia Process — **Thérèse G. Lee**

**4:06 Paper 390c:** Dynamic Simulations and Optimization for Chemical Plant Turnaround Flare Minimization Via Multi-Plant Material Exchange — **Yiling Xu**, Sujing Wang, Thomas Ho, Qiang Xu

**4:24 Paper 390d:** Study for the Optimal Operation of Natural Gas Liquid Recovery and Natural Gas Production — **Mozammel Mazumder**, Qiang Xu, Srinivas Palanki

**4:42 Paper 390e:** Energy Optimization of a Low-Temperature Distillation System for Upgradation of High CO<sub>2</sub> Content Natural Gas — **Usman Hamid**, **Muhammad Faheem**

**5:00 Paper 390f:** Advancing Export Terminal Technology: An Optimized Process for the Refrigeration of Cryogenic Hydrocarbons — **Martin Rosetta**, Komal Patel

**5:18 Paper 390g:** Microwave-Assisted Conversion Of Heavy Oils to Light Olefins — **Faisal M. Alotaibi**

**5:36 Paper 390h:** A Novel, Environmentally Benign Supercritical CO<sub>2</sub>-Ethanol System to Produce High-Yield Carbon Fiber Pre-Precursor from Power River Basin Coal — **Wenyang Lu**, Tongtong Wang, Xin He, Kaidi Sun, Maohong Fan

**(391) Continuous Processing Technologies Applied in Drug Substance Manufacturing II**  
**Tuesday, Oct 30, 3:30 PM**  
Westin Convention Center, Somerset

Shujauddin M. Changi, Chair  
Brian M. Wyvratt, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 391a:** A Comparative Study of Residence Time Distribution and Cooling Crystallization in a Continuous Dynamic/Oscillatory Baffle Crystallizer Versus a Stirred Tank — **Claire Yiqing Liu**, Alastair Barton, Paul Firth, Jonathon Speed, Dan Wood, Zoltan K. Nagy

**3:52 Paper 391b:** Design of Fluoropolymer Membrane Systems for the Dehydration of Organic Solvents for Use in Continuous Flow Chemistry Pharmaceutical Processes — **Hannah Murnen**, Evan Sohodski, Sudip Majumdar, Bryan Feyock

**4:14 Paper 391c:** Advanced, Material-Aware Model Predictive Control Strategies for Evaporation Processes in the Pharmaceutical Industries — **Ioana Nascu**, Nikolaos A. Diangelakis, Salvador García-Muñoz, Efstratios N. Pistikopoulos

**4:36 Paper 391d:** Applications of Continuous Isolation and Drying in Pharmaceutical Manufacturing — **Christopher S. Polster**, Alexander M. Heller

**4:58 Paper 391e:** Development of a Novel Drying Technology for Drying of Wet API's — **Manuel Zettl**, Manuel Kreimer, Isabella Aigner, Markus Krumme, Thomas Mannschott, Peter van der Wel, Johannes G. Khinast

**5:20 Paper 391f:** Possibilities and Limitations of Static Mixers in Precipitating Environments — **Manuel Zettl**, Manuel Kreimer, Isabella Aigner, Markus Krumme, Thomas Mannschott, Peter van der Wel, Johannes G. Khinast

**5:42 Paper 391g:** Coupling Flow Synthesis and Formulation By Electrospinning — **Andrés Domokos**, Attila Balogh, Balázs Farkas, Balázs Dérmuth, Hajnalka Pataki, Zsombor K. Nagy, György Marosi

**(392) Cybersecurity**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 333

Helen Durand, Chair  
Panagiotis D. Christofides, Co-Chair  
Hoda Mehrpouyan, Co-Chair

**Sponsored by:** Next-Gen Manufacturing

**3:30 Paper 392a:** Designing Difficult-to-Cyberattack Process Control Systems — **Helen Durand**

**3:50 Paper 392b:** Cyber Security of Model Predictive Control Systems for Chemical Processes — **Zhe Wu**, Junfeng Zhang, Yannong Li, Helen Durand, Panagiotis D. Christofides

**4:10 Paper 392c:** Keynote Talk: Technology Development for Cybersecure Fossil Power Generation — **Briggs White**

**4:45 Paper 392d:** Keynote Talk: Cybersecurity of Critical Infrastructures — **David Foose**

**5:20 Paper 392e:** Keynote Talk: Cybersecurity Realities in Industrial Control System Environments — **Kenny Mesker**

**(393) Data Driven Modeling and Decision Making**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 410

B. Erik Ydstie, Chair  
Bethany Nicholson, Co-Chair

**Sponsored by:** Data and Information Systems

**3:30 Paper 393a:** A Metaheuristic Approach to Best Subset Selection for the Development of Regression-Based Surrogate Models — **Owais Sarwar**, Nick Sahinidis

**3:49 Paper 393b:** Data-Driven Stochastic Robust Optimization for Process Operation Under Uncertainty — **Chao Ning**, Fengqi You

**4:08 Paper 393c:** Uncertainty Quantification and Stochastic Programming Strategies for Energy Market Participation — **Xian Gao**, Steven Atkinson, **Alexander W. Dowling**

**4:27 Paper 393d:** Predicting Future Production for Unconventional Resources: A Data-Driven Approach — **Sunit Mathur**, Matteo Marongiu-Porcu, **Michael Nikolaou**

**4:46 Paper 393e:** Distributed Approximate Dynamic Programming (dADP) for Data-Driven Optimal Control of Nonlinear Systems — **Wentao Tang**, Prodomos Daoutidis

**5:05 Paper 393f:** Data-Driven Evolution Equation Reconstruction for Parameter-Dependent Nonlinear Dynamical Systems — **David Sroczynski**, Or Yair, Felix Dietrich, Ronen Talmon, Ioannis G. Kevrekidis

**5:24 Paper 393g:** Integrated Data-Driven Monitoring & Explicit Fault-Aware Control of Chemical Processes: An Adaptive Approach for Smart Operation — **Melis Onel**, Baris Burnak, Efstratios N. Pistikopoulos

**5:43 Paper 393h:** Why Plant Operations Are Unstable after All the Design and How Data Science Can Help — **S. Joe Qin**, Yining Dong

**(394) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 317

Fengqi You, Chair  
Gerardo J. Ruiz-Mercado, Co-Chair  
Debalina Sengupta, Co-Chair

**Sponsored by:** Sustainable Energy

**3:30 Paper 394a:** Cost-Competitive Electrolysis-Based Hydrogen Under Current U.S. Electric Utility Rates — **Omar J. Guerra**, Joshua Eichman, Bri-Mathias S. Hodge, Jennifer Kurtz

**4:00 Paper 394b:** Environmental and Economic Analysis for Sustainable Management of Livestock Waste — **Apoorva Sampat**, Gerardo J. Ruiz-Mercado, Victor M. Zavala



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.

**4:30 Paper 394d:** Multi-Objective Planning Approach for Supply Chains Based on Biomass Processing By a Sequential Methodology Via Geographic Information System and Mathematical Programming — **José Ezequiel Santibañez-Aguilar, Francisco José Lozano, Diego Fabián Lozano-García, Antonio Flores-Tlacuahuac**

**5:00 Paper 394e:** Accounting for Spatial Variability of Ecosystem Services in Sustainable Supply Chain Design — **Tapajyoti Ghosh, Bhavik R. Bakshi**

**(395) Developments in Biorefineries**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 316

Eric C. D. Tan, Chair  
Kok Siew Ng, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**3:30 Paper 395a:** Techno-Economic Analysis and Life-Cycle Assessment for Gas Phase Catalytic Oxidation of Lignin to Produce Phenolic Compounds — **Eric C. D. Tan, Matthew M. Yung, Calvin Mukarakate, Mark Nimlos, Michael B. Griffin, Seonah Kim**

**3:50 Paper 395b:** Kinetics of Pyrolysis-GCMS and Thermogravimetric Analysis of Oil-Laden Biomass Intermediate from Flashed-Hydrolyzed Microalgae — **Alexander Asiedu, Sandeep Kumar**

**4:10 Paper 395c:** Framework for Multi-Scale Modeling and Dynamic Simulation of a Biorefinery — **Tobias Ploch, Xiao Zhao, Niklas Tenhaef, Jonathan Hüser, Eric von Lieres, Ralf Hannemann-Tamás, Uwe Naumann, Wolfgang Wiechert, Alexander Mitsos, Stephan Noack**

**4:30 Paper 395d:** Solar Powered Biomass Pyrolysis: A Carbon Neutral Pathway for Producing Fuels and Chemicals — **Asif Hasan Rony, Dengfeng Qin, Tongtong Wang, Maohong Fan**

**4:50 Paper 548x:** A Total Site Synthesis (TSS) Model for the Selection, Integration and Planning of Multiple-Process and Multiple-Feedstock Biorefineries — **Konstantinos A. Pyrgakis, Antonis C. Kokossis**

**5:10 Paper 395f:** Optimal Bio-Refinery Configuration Using Economic Metrics and Environmental Impacts Considering Supply, Demand and Process Uncertainties — **Abhay Athaley, Yue Zhang, Marianthi Ierapetritou**

**(396) Diffusion in Polymers**

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 327

Narayan Ramesh, Chair  
Ahmed E. Ismail, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 396a:** The Molecular Mechanism of Gas Diffusion in Polymers — **Sanat K. Kumar**

**4:00 Paper 396b:** Dissolution of Semicrystalline Polymers: Effects of Solvent Diffusion, Polymer Chain Decrystallization and Disentanglement, and Particle Size — **Mohammad Ghasemi, Marina Tsiannou, Paschalis Alexandridis**

**4:15 Paper 396c:** Examination of the Payne Cell Method for the Evaluation of Permeation, Diffusion, and Solubility Coefficients — **John M. Zielinski, Sacide Alsoy Altinkaya, Armando R. Garcia**

**4:30 Paper 396d:** A Novel Chromogenic Technique for Measuring Nanoscopic Diffusion Phenomena in Polymers — **Calen Leverant, Peng Jiang**

**4:45 Paper 396e:** Study of Concentration Dependent Diffusion Coefficient of Lithium Salt in Block Copolymer — **Kyoungmin Kim, Daniel T. Hallinan Jr.**

**5:00 Paper 396f:** Interplay of Local Chain Dynamics and Viscoelastic Properties on Liquid Water Transport in Ionomer Nanocomposite Membranes — **Apoorv Balwani, Antonio Faraone, Eric M. Davis**

**5:15 Paper 396g:** Influence of Polymer Backbone Rigidity on the Water and Ion Transport Properties of Low Water Content Membrane Polymers — **Kevin Chang, Andrew Korovich, William Morris, Tianyi Xue, Louis Madsen, Bradley Frieberg, Christopher M. Stafford, Geoffrey M. Geise**

**5:30 Paper 396h:** From 1D to 3D: Combined Experimental and Triple-Mode Sorption Modeling Study of Sorption and Transport in Materials — **Hom Sharma, Yunwei Sun, Elizabeth Glascoe**

**5:45 Paper 396i:** Co-Permeation of Alcohols in Hydrated Polymer Membranes — **Bryan S. Beckingham, Breanna M. Dobyms**

**(398) Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)**

**Tuesday, Oct 30, 3:30 PM**

Westin Convention Center, Allegheny Grand Ballroom II

Michael C. Jewett, Chair  
Shelly Peyton, Co-Chair  
Rajanikanth Vadigepalli, Co-Chair

**Sponsored by:** Food, Pharmaceutical & Bioengineering Division

**3:30 Paper 398a:** Dynamic Modulation of Protein Functions by Strand Displacement — **Wilfred Chen**

**4:30 Paper 398b:** Fabrication of Cellulosic Fibers for use as Functional Materials — **Ping Wang**

**4:50 Paper 398c:** Nanomaterials for Combination Therapies and Immunomodulation — **Surya Mallapragada**

**5:10 Paper 398d:** A Sense of Balance: Exploring the Role of Metabolic Pathway Modularization in the Microbial Production of Chemicals — **Mattheos A. G. Koffas**

**5:30 Paper 398e:** Repairing the Brain After Stroke: a Biomaterials Strategy — **Tatiana Segura**

**(399) Electrocatalysis and Photoelectrocatalysis VI: Biomass Processing and Ammonia Synthesis**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 401

Timothy Van Cleve, Chair  
Elizabeth J. Biddinger, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 399a:** Adsorption of Organics and Nitrate on Pt Electrodes for Electrochemical Reduction Reactions — **Nirala Singh, Udishnu Sanyal, Danielle Richards, Jin-Xun Liu, John L. Fulton, Charles T. Campbell, Johannes A. Lercher, Bryan Goldsmith**

**3:48 Paper 399b:** Mechanistic Insights into Selective Hydrogenation of Furfural over Metal Electrodes — **Xiaotong Chadderdon, David Chadderdon, John Matthiesen, Jean-Philippe Tessonnier, Wenzhen Li**

**4:06 Paper 399c:** Impact of Phenol on the Electrocatalytic Hydrogenation of Carbonyl Compounds on Metal Catalysts — **Udishnu Sanyal, Katherine Koh, Laura Meyer, Jamie Holladay, Oliver Gutiérrez, Johannes A. Lercher**

**4:24 Paper 399d:** Electro-Oxidation of Furans to Value-Added Chemicals — **Alex Roman, J. Will Medlin, Adam Holewinski**

**4:42 Paper 399e:** Low Energy Electrochemical Oxidation of Waste Lignin on Non-Precious PbO<sub>2</sub>/MWNTs Electrocatalyst for Simultaneous Generation of Value-Added Chemicals and Hydrogen — **Fazel Bateni, John Staser**

**5:00 Paper 399f:** Metal Nitride-Type Cathode Catalysts for Electrocatalytic Ammonia Production — **Seval Gunduz, Dhruva Jyoti Deka, Doruk Dogu, Katja E. Binkley Meyer, John McGrogan, Anne Co, Umit S. Ozkan**

**5:18 Paper 399g:** Selective Hydrogenations in Proton Exchange Membrane Reactor — **Sarah Carl, Krysta Waldrop, Peter N. Pintaur, Levi T. Thompson**

**5:36 Paper 399h:** Rational Design of Metal Electrocatalysts for Ambient Ammonia Synthesis — **Xiaofeng Feng**

**(400) Electrochemical Engineering: Industry-Relevant Problems and Solutions**

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 306

John Staser, Chair

**Sponsored by:** Electrochemical Fundamentals

**3:30 Paper 400a:** High Speed Imaging of Bubble Flows in Membraneless Electrochemical Cells — **Jonathan Davis, David Brown, Xueqi Pang, Daniel Esposito**

**3:50 Paper 400b:** Polystyrene-Block-Poly(ethylene-*ran*-butylene)-Block-Polystyrene Triblock Copolymer Separators for a Vanadium-Cerium Redox Flow Battery — **Zhongyang Wang, Javier Parrondo, Vijay Ramani**

**4:10 Paper 400c:** Electrochemical Oxidation of Lignin for Production of Value-Added Chemicals Using a Flow Electrochemical Reactor — **Raziyeh Ghahremani, John Staser**

**4:30 Paper 400d:** Depolymerization of Waste Lignin to Valuable Low Molecular Weight Aromatic Compounds Via a Continuous Electrochemical Reactor — **Mahtab Naderinasrabadi, John Staser**

**4:50 Paper 400e:** Mass Transfer and Current Distribution of Hydrodynamic Electroplating Test Cells — **Tsung-Wei Zeng, Shi-Chern Yen**

**5:10 Paper 400f:** Fundamental Drivers and Mechanisms for Dendritic Zn Growth, Electrolyte Leakage and Hydrogen Gassing in Zn-MnO<sub>2</sub> Batteries — *Ehsan Faegh, Travis Omasta, Matthew Hull, Micheal Zuraw, William E. Mustain*

**5:30 Paper 400g:** Study of the Electrochemical Growth of Charge Transfer Complex Nanowires and Their Application in Gas Sensing — *Mohamed Kilani, Disni Gunasekara, Long Luo, Guangzhao Mao*

**5:50 Paper 400h:** Electrochemical Atomic Layer Deposition and Etching of Metals for Applications in Semiconductor Nano-Manufacturing — *Kailash Venkatraman, Yukun Gong, Rohan Akolkar*

#### (401) Emerging Trends in Life Cycle Analysis

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 315

Vikas Khanna, Chair  
Fengqi You, Co-Chair

**Sponsored by:** General

**3:30 Paper 401a:** A Model-Based Life Cycle Analysis of Hydrotreated Renewable Jet Fuel (HRJ) from Oilseed Feedstocks Replacing Fallow in the U.S. Northern Great Plains — *Rui Shi, David W. Archer, Krishna Pokharel, Matthew Pearson, Kristin C. Lewis, Suchada Ukaew, David R. Shonnard*

**3:50 Paper 401b:** Towards Systematic Design on Life Cycle Assessment Models By Accounting for Uncertainty and Network Complexity — *Tapajyoti Ghosh, Bhavik R. Bakshi*

**4:10 Paper 401c:** Designing with the System in Mind: Life Cycle Assessment of Nano-Enabled Agrochemicals — *Leila Pourzahedi, Madelyn Pandorf, Dwarakanath Ravikumar, Julie Zimmerman, Thomas Seager, Thomas Theis, Paul Westerhoff, Leanne Gilbertson, Gregory V. Lowry*

**4:30 Paper 401d:** Environmental Life Cycle Assessment of Peracetic Acid Application in the Pulp and Paper Industry — *Darlene Echeverria, Richard Venditti, Hasan Jameel, Yuan Yao*

**4:50 Paper 401e:** Transforming the Circular Economy with the Value Web Model – a Multi-Objective Spatio-Temporal MILP Model for Planning, Design & Operation of Integrated Circular Value Chains — *Sheila Samsatti*

**(402) Enabling and Advanced Formulations in Drug Product Processing II: Focus on Stability**  
**Tuesday, Oct 30, 3:30 PM**  
Westin Convention Center, Washington  
Gulsad Kucuk, Chair  
John Peragine, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 402a:** In Situ Studies of Phase Separation in Amorphous Solid Dispersions (ASDs) Using the QCM-D — *Mark A. Isbell, Geoff G. Z. Zhang, Jerry Y. Y. Heng*

**3:51 Paper 402b:** Mathematical Models for the Stability of Atropisomer-Forming Drug Substance in a Spray-Dried Dispersion Formulation — *Jose Tabora, Thomas M. Razler, Brian He*

**4:12 Paper 402c:** Study of Nimesulide Recrystallization Kinetics By Particle Sizing, Microscopy, and Raman — *Tim E. Alcacio, Gregor Hsiao*

**4:33 Paper 402d:** Revealing Polymorphic Phase Transformations in Polymer-Based Hot Melt Extrusion Processes — *Jose Hernandez Espinell, Vilma Lopez-Mejias, Torsten Stelzer*

**4:54 Paper 402e:** Development of a Tablet Manufacturing Line Via Hot-Melt Extrusion and Strand Pelletization — *Theresa R. Hörmann, Otto Scheibelhofer, Jakob Rehr, Adrian Funke, Amrit Paudel, Johannes G. Khinast*

**5:15 Paper 402f:** Exploring Mesoporous Supports As a Means to Separate Physical Property Control from Crystallization — *Christopher S. Polster, Justin Burt, Jeremy Merritt, Mark Polizzi, Dale E. Greenwood, Aktham Aburub*

**5:36 Paper 402g:** Generation of Stable Nanobubbles Following Reconstitution of Lyophilized Protein Formulations: Effects of Excipient Structure on Nanobubble Formation — *Jared Snell, Theodore W. Randolph*

**(403) Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 308

Jeffrey Errington, Chair  
Jim Pfandtnr, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**3:30 Paper 403a:** Programmable Assembly of Multiflavored DNA-Functionalized Particles — *Jeetain Mittal*

**4:10 Paper 403b:** Coarse-Grained Models for Understanding Transport in Soft, Crowded Matrices — *Jeremy C. Palmer*

**4:30 Paper 403c:** Engineering Pathways across Biological Barriers — *Shikha Nangia*

**4:50 Paper 403d:** Methodologies for Enhanced Unbiased Sampling of the Free Energy Landscapes of Proteins — *Diwakar Shukla*

**5:30 Paper 403e:** Taming the Complexity of a Messy Solution Process to Find Better Materials for Solar Cells: A Bayesian Optimization-Guided Route to Better Bouillabaisse — *Paulette Clancy*

#### (404) Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 320

Eunsung Kan, Chair  
Ramesh Chawla, Co-Chair  
Robert W. Peters, Co-Chair

**Sponsored by:** Solid and Hazardous Waste

**3:30 Paper 404a:** Combustion Analysis of Trash to Tank Fuel Derived from Plastic Waste — *Chandni Joshi, Jeffrey R. Seay*

**3:51 Paper 404b:** Atatad Heat Accumulation in Countercurrent Flow, Continuous Phase Sludge Treatment Process to Class a Fertilizer — *Sarah Johnson*

**4:12 Paper 404c:** Development and Deployment of Advanced Technology for Mswi Fly Ash Stabilization and Utilization Via High-Gravity Carbonation Process — *Tse-Lun Chen, Shu-Yuan Pan, Pen-Chi Chiang, Yi-Hung Chen, Kinjal Shah*

**4:33 Paper 404d:** Investigation on CO<sub>2</sub> co-Gasification of Horticultural Waste and Sewage Sludge for Energy Production: Effects of Temperature, Ash Content and CO<sub>2</sub> flow Rate — *Ye Shen, Xiang Kan, Chi-Hwa Wang*

**4:54 Paper 404e:** Waste Management in International Airports: A Case Study of Astana Airport — *Gaukhar Balbayeva, Yerbol Sarbassov, Christos Venetis, Tokmyn Sagalova, Diyar Tokmurzin, Berik Aiyembetov, Bexultan Abylkhan, Almira Yagofarova, Edward Anthony, Vassilis J. Inglezakis*

**5:15 Paper 404f:** Comparison between Multi-Stage and Single Stage Microalgaedewatering Processes — *Hazim Qiblawey, Fares Almomani*

**5:36 Paper 404g:** Improving Biogas Production from Agricultural Waste By Photo-Fenton Process — *Rahul Bhosale, Anand Kumar, Fares Almomani*

#### (405) Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 413

Steven R. Saunders, Chair  
He Jing, Co-Chair

**Sponsored by:** Nanoparticles

**3:30 Paper 405a:** Ceria Nanoparticle Dissolution and Stability in Acidic Aqueous Environments — *Matthew L. Hancock, Robert Yokel, Eric A. Grulke*

**3:50 Paper 405b:** Probing Peptoid-Carbon Nanotube Coatings for Biological Imaging — *Linda Chio, Markita Landry*

**4:10 Paper 405c:** Synthesis, Characterization, and Interfacial Properties of Lignin Coated Iron Oxide Magnetic Nanoparticles in Aqueous Solutions — *Frankie Petrie, Mohammad J. Hassan, Esteban E. Ureña-Benavides, Erick S. Vasquez*

**4:30 Paper 405d:** Investigation of Interactions between Magnesium Silicate Particles and Diamond-like Carbon Surface By Atomic Force Microscopy — *Vipada Dokmai, Varong Pavarajarn*

**4:50 Paper 405e:** Polymer-Metal Composite Nanoparticles Via Vapor Phase Deposition Processes Onto Liquid Substrates — *Mark De Luna, Prathamesh Karandikar, Malancha Gupta*



**5:10 Paper 405f:** Controlling Surface Morphology and Spatial Distribution of Active Nanoinclusions in Functional Coatings Via Air-Controlled Electrospray Process — **Mounica Jyothi Divvela, Yong Lak Joo**

**(406) Industrial Application of Computational and Numerical Approaches to Particle Flow**

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 415

Lev Davydov, Chair  
Madhusudhan Kodam, Co-Chair

**Sponsored by:** Fluidization and Fluid-Particle Systems

**3:30 Paper 406i:** Role of Computational Modeling in Fluid Catalytic Cracking Design — **Raj Singh**

**3:48 Paper 406b:** Direct Numerical Simulations of Flow Around Assemblies of Non-Spherical Particles and the Investigation of Voidage Effects — **Johan T. Padding, Sathish K.P. Sanjeevi**

**4:06 Paper 406c:** Detailed Analysis of a Large-Scale Wurster Coating Process — **Thomas Forgeber, Martina Trogrlic, Dalibor Jajcevic, Pankaj Doshi, Mary T. am Ende, Alan Carmody, Johannes G. Khinast, Avik Sarkar**

**4:24 Paper 406d:** MFIX-Exa: A CFD-DEM Code for Exascale Computer Architectures — **Madhava Syamlal, Jordan Musser, Ann Almgren, John Bell, Christine Hrenya, Thomas Hauser, Peiyuan Liu**

**4:42 Paper 406e:** Simulation As a Tool for Learning from Historical FCC Regenerator Operations — **John Pendergrass, Peter Blaser, Samuel Clark**

**5:00 Paper 406f:** Evaluation of Filtered Two Fluid Models Against Data from an Industrial Scale Fluidized Bed Reactor — **Henri Cloete, Schalk Cloete, Thomas Gurker, Günter Gronald, Shahriar Amini**

**5:18 Paper 406g:** Finding the Preferred Safe Operating Condition of a Fluidized Bed Incinerator to be Used for the Disposal of Waste Explosives — **Sunghyun Cho, Hyungtae Cho, Chanho Park, Jinwoo Park, Hyoungsoo Kim, Il Moon**

**5:36 Paper 406h:** Three Dimensional CFD Simulation of Two-Phase Flow in Pilot Plant Dryer — **Hossein Hassanzadeh, Masoud Asadiagheri, Mostafa K. Moraveji, Mahdi Hozhabri Namin, Ali Nabizadeh**

**(407) In Honor of the 2018 CRE Young Investigator Award Winner (Invited Talks)**

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 405

Kurt VandenBussche, Chair  
Lars C. Grabow, Co-Chair  
Yuriy Román-Leshkov, Co-Chair  
Paul J. Dauenhauer, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 407a:** Introductory Remarks By the CRE Young Investigator Award Committee — **Robert W. McCabe, Kurt VandenBussche, Lars C. Grabow**

**3:40 Paper 407b:** Breaking the Barriers in Lignin Upgrading Using a Catalytic Funneling Strategy — **Yuriy Román-Leshkov**

**4:10 Paper 407c:** How Can Catalysis Enable the Reduction of CO<sub>2</sub> Emissions By the Fuels and Chemicals Industries? — **Alexis T. Bell**

**4:30 Paper 407d:** Development of New Flow Reactors and Their Application for Rhodium-Catalyzed C-H Activation in Organic Synthesis — **Chunjae Yoo, Eric G. Moschetta, Kathryn M. Chopiga, Daniel Rackl, Solyman Negretti, Nicholas Brunelli, Ryan Lively, Huw M. L. Davies, Christopher W. Jones**

**4:50 Paper 407e:** Metal Catalysts for Cooperative Activation of Cellulose — **Paul J. Dauenhauer**

**5:20 Paper 407f:** New Methods for the Synthesis of Zeolite and Metal-Organic-Framework Catalysts and Membranes — **Michael Tsepatsis**

**5:40 Paper 407g:** From First Principles to Chemical Manufacturing of Renewable Chemicals — **Dionisios G. Vlachos**

**(408) Integrated Process Engineering and Economic Analysis**

**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 318

Yizu Zhu, Chair  
Julie N. Renner, Co-Chair  
Mike Dou, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**3:30 Paper 408a:** Conceptual Process Design and Economic Analysis of a Diving-Wall Distillation Sequence for Catalyst Reforming Unit — **Weixuan Zhu, Xiong Zou, Haotian Ye, Yang Yang, Hong-guang Dong**

**3:47 Paper 408e:** Guidelines for Techno-Economic Assessment of Carbon Capture and Utilization Technologies — **Arno W. Zimmermann, Johannes Wunderlich, Georg A. Buchner, Annika Marxen, Katy Armstrong, Stavros Michailos, Henriette Naims, Peter Styring, Prof. Dr. Reinhard Schomäcker**

**4:04 Paper 408j:** Gas Capture by Ionic liquids — **Xiaochun Zhang, Suojing Zhang**

**4:21 Paper 408d:** Thermoeconomic Optimization of Reverse Brayton Cycle Based Cryocooler for HTS Power Transmission Cable — **Aman Dhillon, Parthasarathi Ghosh**

**4:38 Paper 408c:** Technology Readiness Levels As a Framework for Techno-Economic Assessment — **Georg A. Buchner, Arno W. Zimmermann, Annika Marxen, Kai J. Stepputat, Arian E. Hohgräve, Reinhard Schomäcker**

**4:55 Paper 408f:** Techno-Economic Modeling and Optimization of Catalytic Reactive Distillation for Bio-Oil Upgradation — **M. Arif Khan, Yusuf G. Adewuyi**

**5:12 Paper 408g:** Superstructure Optimization of Membrane-Based Carbon Capture Systems — **Miguel A. Zamarripa, Samir Budhathoki, Olukayode Ajayi, Janice A. Steckel, Christopher E. Wilmer, Michael S. Matuszewski, David C. Miller**

**5:29 Paper 408k:** Making Hydrogen from Water with a Protein Organized Electrode: Ultra-High Utilization of Noble Metal in Proton Exchange Membrane Electrolysis for Capital Cost Reduction — **Nuttanit Pramounmat, Julie N. Renner**

**5:46 Paper 408i:** Design Optimization and Economic Evaluation of LNG/NGL Integrated Processes Under Lean Feed Composition — **Chunhe Jin, Youngsub Lim**

**6:03 Paper 408h:** Techno-Economic Analysis of Integrated Low Grade Waste Heat Recovery Combined Cycle for Power, Heating, Cooling, and Desalination — **Wai Mun Chan**

**(409) Interfacial Transport Phenomena**

**Tuesday, Oct 30, 3:30 PM**  
Omni William Penn Hotel, Conference Center A

Vivek Sharma, Chair  
Sven H. Behrens, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 409a:** Nanoparticle Adsorption Dynamics at Fluid Interfaces — **Xiaoqing Hua, Joelle Frechette, Michael A. Bevan**

**3:45 Paper 409b:** Transport of Lipid Amphiphiles to Fluid Interfaces from a Vesicle Dispersion — **Jennifer Staton, Stephanie R. Dungan**

**4:00 Paper 409c:** Dynamic Adsorption and Dynamic Surface Tension Measurements of Ionic Surfactants Using Maximum Bubble Pressure Tensiometry — **Camilla U. Ortiz, Carina Martinez, Norman Moreno, Vivek Sharma**

**4:15 Paper 409d:** The Effect of Micro-Post Configuration on Interfacial Mass Transfer in a Milli-Scale Reactor — **Milad Mottaghi, G. D. Stefanidis, Simon Kuhn**

**4:30 Paper 409e:** Controlling Crack Evolution in Drying Suspensions — **H. Jeremy Cho, Nancy B. Lu, Sujit S. Datta**

**4:45 Paper 409f:** Evaporative Suppression of Film Instability in Pure and Binary Mixtures — **Dipin Pillai, Ranga Narayanan**

**5:00 Paper 409g:** Spontaneous Imbibition and Forced Wetting in Closed Square Capillaries and Open Rectangular Grooves — **Vignesh Thammanna Gurumurthy, Daniel Rettenmaier, Ilia Roisman, Cameron Tropea, Stephen Garoff**

**5:15 Paper 409h:** Studying the Interface of Warm Mix Asphalts — **Yi-lun Lee, Liqun Zhang, Xiong Yu, Jianying Hu**

**5:30 Paper 409i:** Numerical Simulation for Multiple Bubble Interactions in Low Temperature Fluids — **Joydip Mondal, Arpit Mishra, Rajaram Lakkaraju, Parthasarathi Ghosh**



#### (410) LGBTQ+ Inclusion in Engineering

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center,  
Spirit of Pittsburgh B  
Stephanie Farrell, Chair  
Gayle Gibson, Co-Chair

**Sponsored by:** Diversity & Inclusion

**3:30 Paper 409a:** Workshop & Training on Being a Better Ally of LGBTQ+ Engineers — **Stephanie Farrell**

**4:45 Paper 409b:** Panel of Leaders Discuss Their Experiences with LGBTQ+ Inclusion — **Gayle Gibson, Deborah Grubbe, Eric Reiner, Jim Fitterling**

#### (411) Lignocellulosic Materials

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center,  
325

Manju Misra, Chair  
Amar K. Mohanty, Co-Chair

**Sponsored by:** Forest and Plant Bioproducts Division

**3:30 Paper 411a:** Furan Production from Biomass Hydrolysates: Scale-up of a Novel, High-Yield "Sire" Process — **Ravikumar Gogar, Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi**

**3:55 Paper 411b:** A Novel and Green Approach in Engineering Transparent and Homogenous Cellulose Nanocrystal-Lignin UV Protection Films — **Mahesh Parit, Partha Saha, Virginia Davis, Zhihua Jiang**

**4:20 Paper 411c:** Effect of Activation Temperature on Oxygen Functional Groups and Corresponding Electron Exchange Capacities on Hydrochar — **M. Toufiq Reza, Nepu Saha, Akbar Saba**

**4:45 Paper 411d:** Graphene from Biomass — **Manju Misra, Amar K. Mohanty**

**5:10 Paper 411e:** The Effects of Hydrolyzed Lignocellulose Materials on the Performance of Water-Based Drilling Fluids — **Jimoh K. Adewole, Musa O. Najimu, Ahmad Adewunmi**

**5:35 Paper 411f:** Oxidative Pretreatment Process of Sugarcane Bagasse Assisted By Hydrodynamic Cavitation — **Terán Hilaes Ruly, M.Ajaz Ahmad, Ayyaz Ahmad**

#### (412) Microfluidic and Nanoscale Flows: Separations & Particulates

**Tuesday, Oct 30, 3:30 PM**

Omni William Penn Hotel, Frick

Aditya S. Khair, Chair  
Hadi Mohammadigoushki, Co-Chair

**Sponsored by:** Fluid Mechanics

**3:30 Paper 412a:** Coarse-Grained Simulations of Trapping and Separation Using Microfluidic Flows and Fields — **Patrick T. Underhill**

**4:00 Paper 412b:** Flow of Wormlike Micellar Fluids Around a Sharp Microfluidic Bend: Effects of Branching and Shear-Banding — **Yiran Zhang, Hadi Mohammadigoushki, Margaret Y. Hwang, Susan J. Muller**

**4:15 Paper 412c:** Shear-Thinning Behavior of Supercooled Water inside Small Nanotubes and Shear Effect on the Tetrahedral Structure — **José Cobeña, Muhammad Sahimi**

**4:30 Paper 412d:** Rapid Separation of  $\lambda$ DNA Digests in Entangled Micelle Networks — **Lingxiao Yan, Kimberly Hui, Jim Schneider**

**4:45 Paper 412e:** Assembly of Protocell-like Vesicles Via Chaotic Convective Flow in Micro-Scale Hydrothermal Pores — **Vijay Ravisankar, Yassin A. Hassan, Victor M. Ugaz**

**5:00 Paper 412f:** Differentiating Effects of Geometry and Fluid Rheology on the Dispersion of Particles in 2-D Microfluidic Porous Media Via Microfluidic Experiments and Computations — **Jack Jacob, Deepak Mangal, Jeremy C. Palmer, Ramanan Krishnamoorti, Jacinta C. Conrad**

**5:15 Paper 412g:** Dispersion in Steady Two-Dimensional Flows through a Parallel-Plate Channel — **Henry C. W. Chu, Stephen Garoff, Todd M. Przybycien, Robert D. Tilton, Aditya S. Khair**

**5:30 Paper 412h:** Particle Transport and Damage in Confined Channels — **Alexander Zinchenko, Cassandra Giammo, Brian Robb, Robert Davis**

**5:45 Paper 412i:** Migration and Equilibrium Configuration of Double Emulsion Drops in Microfluidic Channels — **Sadeh Dabiri, Sangkyu Kim**

#### (413) Microreaction Engineering II

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center,  
404

Milad Abolhasani, Chair  
Andrew Teixeira, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 413a:** Open Source Controls, Cloud Computing and Paradigm Changes in Laboratory-Scale Reactor Control — **Benjamin Rizkin, Ryan L. Hartman**

**3:51 Paper 413b:** Two-Phase Microreactor Design for the Reactive Extraction of Biomass Derivatives — **Pierre Desir, Basudeb Saha, Dionisios G. Vlachos**

**4:12 Paper 413c:** Alloy Catalysis Spanning Composition Space — **Irem Sen, Petro Kondratyuk, Andrew J. Gellman**

**4:33 Paper 413d:** Microfluidic Approaches for Accessing Thermodynamic Properties of Fluid Systems — **Théo Gavoille, Nicolas Pannacci, Ghislain Bergeot, Samuel Marre**

**4:54 Paper 413e:** Hydrogenation of Renewable Oil in Microscale-Based Reactor — **Dan Huang, Frederick Atadana, Matthew Young Cobylyn, Nichaporn Sirimungkalakul, Thana Sornchamni, Goran N. Jovanovic**

**5:15 Paper 413f:** Converting Biogas to Liquid Fuels By Low Energy Electrical Corona Discharge Processes — **Yu Miao**

**5:36 Paper 413g:** Microenvironment Effect on Reaction Kinetics within Self-Assembled Polymer Nanoreactors — **Andrew Harrison, Tien Vuong, Michael Zeevi, Christina Tang**

#### (414) Mixing and Segregation of Particulates

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center,  
414

Aaron Morris, Chair  
Yi Fan, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**3:30 Paper 414a:** Coupling a Continuum Granular Segregation Model with a Flow Model Incorporating Granular Rheology — **Richard M. Lueptow, Hongyi Xiao, Jinhui Yan, Gregory J. Wagner, Julio M. Ottino, Paul B. Umbanhowar**

**3:48 Paper 414b:** Modeling Granular Material Segregation Using a Finite Element Method and Advection-Diffusion-Segregation Equation Multi-Scale Model — **Yu Liu, Marcial Gonzalez, Carl Wassgren**

**4:06 Paper 414c:** Continuous Powder Blending inside Twin Screw Extruder — **Daniel Mateo-Ortiz, Dana Alhasson, Bei Chen, Sean Garner, William R. Ketterhagen, Nandkishor Nere, Michael C. Dennis**

**4:24 Paper 414d:** Investigation of the Effect of Baffles on Axial Mixing and Impregnation in a Double Cone Blender — **Yangyang Shen, Aman Rastogi, William G. Borghard, M. Silvina Tomassone**

**4:42 Paper 414e:** Experimental Study of Particle Density Segregation in Granular Shear Flow — **Siying Liu, Joseph J. McCarthy**

**5:00 Paper 414f:** Cohesive Particle Segregation and Granular Rheology — **Siying Liu, Joseph J. McCarthy**

**5:18 Paper 414g:** Estimation and Explanation of Adhesive Mixing Efficiency Via Energy-Based Stick/Bounce Model — **Kai Zheng, Rajesh Davé**

**5:36 Paper 414h:** Segregation of Particles in Electrostatic Environments Where Particles Are Subject to Rebound — **Kerry Johanson**

#### (415) Nanomaterials for Energy Storage II

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center,  
412

Ling Fei, Chair  
Yong Lak Joo, Co-Chair

**Sponsored by:** Nanomaterials for Applications in Energy and Biology

**3:30 Break**

**3:50 Paper 415b:** Synthesis of Carbon Quantum Dots from Ohio-Derived Coal — **Mohammadreza Rostami, John Staser**

**4:10 Paper 415c:** Template-Free Self-Assembly of 3D Graphene/Noble Metal Nanotube Composite Electrocatalysts for Oxygen Reduction Reaction in Fuel Cells — **Enoch Nagelli, Gabrielle Milanesa, F. John Burpo, Kamil Woronowicz, Alexander Mitropoulos**

**4:30 Paper 415d:** Hydrogen Storage in Small PtPd Alloy Nanoparticles: A DFT Study — **Benjamin Wei Jie Chen, Tibor Szilvási, Manos Mavrikakis**

**4:50 Paper 415e:** Salt-Ceramic Composite Electrolytes for Lithium Metal Batteries — **Wonho Lee, Clive Randall, Enrique D. Gomez**

**5:10 Paper 415f:** Atomic Layer Deposition of Nanoscale Solid State Electrolyte for the Next-Generation Energy Storage — **Chuan-Fu Lin, Gary W. Rubloff**

#### (416) Nanoparticles and Health

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 309

Kerry Kelly, Chair  
Nga Lee Ng, Co-Chair

**Sponsored by:** Environmental Aspects, Applications, and Implications of Nanomaterials and Nanotechnology

**3:30 Paper 416a:** Oxidative Potential and Cellular Oxidant Production from Biomass Burning Aerosol — **Nga Lee Ng, Wing-Yin Tuet, Nilmara de Oliveira Alves, Shierly Fok, Dong Gao, Paulo Artaxo, Pérola Vasconcellos, Julie A. Champion, Rodney Weber**

**3:50 Paper 416b:** Brain Imaging Probes Elicit Microglial Inflammatory Responses and Induce Cellular Morphological Changes — **Darwin Yang, Markita Landry**

**4:10 Paper 416c:** Design and Characterization of a New, Portable *in Vitro* Exposure Cassette with Real-Time Monitoring for Aerosol Measurements — **Lynn E. Secondo, Nathaniel J. Wygal, Nastassja Lewinski**

**4:30 Paper 416d:** Surface Chemistry Toxicity Parameters Associated with Combustion Produced PM<sub>2.5</sub> by *in Vitro* Assays — **Randy Vander Wal, Patricia Silveyra, Joshua Muscat, Madhu Singh**

**4:50 Paper 416e:** Effect of Combustion Particle Size on Pathologically Important Responses in Lung Cells — **Kamaljeet Kaur, Raziye Mohammadpour, Cristina Jaramillo, Anne Sturrock, JoAnn S. Lighty, Robert Paine, Christopher Reilly, Hamid Ghandehari, Kerry Kelly**

**5:10 Paper 416f:** Toxicological Screening of Metal Oxide Nanoparticles in Liver Context Demonstrates Apoptosis in Hepatocytes *Versus* Pyroptosis in Kupffer Cells — **Vahid Mirshafiee, Bingbing Sun, Tian Xia, Andre E. Nel**

#### (417) Nanostructured Polymers and Composites

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 330

Stephen M. Martin, Chair  
Joseph F. Stanzione III, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 417a:** Investigating the Swelling Behavior of a Poly(Acrylic acid) Brush Via Quartz Crystal Microbalance w/Dissipation (QCM-D) — **Nisha Hollingsworth, Sabina Wilkanowicz, Ronald G. Larson**

**3:45 Paper 417b:** Monitoring Nanoconfined Inorganic-Polyepoxy-Inorganic Adhesive Interfacial Changes and Molecular Forces during Curing at Various Environmental Conditions — **Roberto C Andresen Eguiluz, Jeffrey Scott, Kai Kristiansen, Howard Dobbs, Thomas R. Cristiani, George Degen, Szu-Ying Chen, Jacob Israelachvili**

**4:00 Paper 417c:** Stimuli-Responsive Thin Coatings Made from Natural Pectins — **Zeinab Veisi, Norma Alcantar, Ryan Toomey**

**4:15 Paper 417d:** Critical Role of Surface Energy in Guiding Crystallization of Solution-Coated Polymer Semiconductor Thin Films — **Erfan Mohammadi, Fengjiao Zhang, Ying Diao**

**4:30 Paper 417e:** Crosslinking Gradients of a Photopolymerized Multifunctional Acrylate Film Control Mechanical Properties — **Matthew L. Hancock, Fugian Yang, Eleanor Hawes, Eric A. Grulke**

**4:45 Paper 417f:** Morphology of Nanocrystalline Domain Reinforced Rubber — **John Meyerhofer, Wenhan Zhao, Yihong Zhao, Li Jia, Mark D. Foster**

**5:00 Paper 417g:** Surface-Initiated Polymerization As a Tool for Chemical Patterning — **Christian W. Pester, Mingxiao Li, Kaila M. Mattson, David Lunn, Gregory Su, Michael Brady**

**5:15 Paper 417h:** Selective Deposition of Fluoropolymers Using Surface Energy Contrast — **Mahdi Mohammadi Ghaleni, Siamak Nejati**

**5:30 Paper 417i:** Evaluation of Three-Dimensional Line-Edge Roughness of Pre-and Post-Dry Etched Line and Space Patterns of Block-Copolymer Lithography — **Shubham Pinge, Durairaj Baskaran, Yong Lak Joo**

**5:45 Paper 417j:** Proton Conductivity of Multi-Acid Ionomer Side Chains Under Confinement — **Seefat Farzin, Shudipto Konika Dishari**

#### (418) Nuclear Applications of Electrochemical Engineering

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 326

Michael Simpson, Chair  
Supathorn Phongikaroon, Co-Chair

**Sponsored by:** Nuclear Engineering Division

**3:30 Paper 418a:** Electrochemical Deposition of Sr and Ba into Liquid Bi from Molten Salt Electrolytes — **Timothy Lichtenstein, Thomas Nigl, Nathan Smith, Hojong Kim**

**3:50 Paper 418b:** Electrochemical Separation of Cs from Molten Salts Using Liquid Metal Electrodes — **Nathan Smith, Thomas Nigl, Hojong Kim**

**4:10 Paper 418c:** Electrochemical Analysis of Bi-Analyte Electrorefiner Salt with High Concentration of UCl<sub>3</sub> — **Chao Zhang, Devin S. Rappeye, Jaron Wallace, Michael F. Simpson**

**4:30 Paper 418d:** Monitoring of Actinide Concentrations in Molten LiCl-KCl Salt Using Alpha Spectroscopy — **Nora Alnajjar, Silvia Padilla, Milan Stika, Joshua Jarrell, Lei Cao, Michael F. Simpson**

**4:50 Paper 418e:** Thermodynamic Properties of Strontium-Lead Alloys Determined By Electromotive Force Measurements — **Thomas P. Nigl, Timothy Lichtenstein, Nathan Smith, Jarrod Gesualdi, Yuran Kong, Hojong Kim**

**5:10 Paper 418f:** Evaluation of Concentrations of Residual Water, Hydroxides, and Oxides in Molten Anhydrous CaCl<sub>2</sub> — **Emma Faulkner, Michael Simpson**

**5:30 Paper 418g:** A Lightweight Betaemitter for Power Applications — **Patrick J. Pinhero**

#### (419) Particulate and Multiphase Flows: Theory & Experiment

**Tuesday, Oct 30, 3:30 PM**

Omni William Penn Hotel, Phipps

Vivek Narsimhan, Chair  
David T. Leighton, Jr., Co-Chair

**Sponsored by:** Fluid Mechanics

**3:30 Paper 419a:** A Higher-Order Slender-Body Theory for Axisymmetric Flow Past a Particle at Moderate Reynolds Number — **Aditya S. Khair, Nicholas G. Chisholm**

**3:45 Paper 419b:** Fast Stokesian Dynamics Simulations with Applications to Brownian Motion and Arbitrarily Shaped Particles — **James Swan, Andrew Fiore**

**4:00 Paper 419c:** Applications of Conformation Tensor-Based Macroscopic Models to Particulate and Multiphase Systems — **Paul M. Mwasame, Norman J. Wagner, Antony N. Beris**

**4:15 Paper 419d:** Modelling of a Resonant Acoustic Mixer Using the Lattice Boltzmann Method with a Free Surface Coupled with the Discrete Element Method — **Ramon E. Lopez, Joseph J. McCarthy**

**4:30 Paper 419e:** Breakage of Single Drops in an Inertial Laminar 2-D Orifice Flow — **Derrick I. Ko, Richard V. Calabrese**

**4:45 Paper 419f:** Gas Holdup and Bubble Behavior in an Upflow Packed Bed Column — **Mahsa Taghavi, Vemuri Balakotaiah**

**5:00 Paper 419g:** Bouncing Particles on a Stratified Coating — **Matthew Tan, Yumo Wang, Joelle Frechette**

**5:15 Paper 419h:** Wall-to-Particle Heat Transfer in Gas-Solids Flows — **Aaron Lattanzi, Xiaolong Yin, Christine M. Hrenya**

**5:30 Paper 419i:** Interplay of Tribocharging and Transport on Particle-Laden Flows — **Jari Kolehmainen, Xiaoyu Liu, Ali Ozel, Sankaran Sundaresan**

**5:45 Paper 419j:** Formation of Fractal Aggregates Among Nanoparticles in Gas-Phase Produced from Non-Equilibrium Plasmas — **Souvik Ghosh, Xiaoshuang Chen, David Buckley, R. Mohan Sankaran, Christopher J. Hogan Jr.**

#### (420) Plenary Session: Multifunctional Biomaterials Addressing Current Healthcare Challenges (Invited Talks)

**Tuesday, Oct 30, 3:30 PM**

Westin Convention Center, Pennsylvania East

Tagbo H.R. Niepa, Chair  
Paul Stoodley, Co-Chair

**Sponsored by:** Microbes at Biomedical Interfaces

**3:30 Paper 420e:** Can Soft-Matter Mechanics Provide New Avenues for Remediating (and even preventing!) Biofilm Infections? — **Vernita D. Gordon**

**3:55 Paper 420b:** Mechanisms of Bacterial Biofilm Growth and Biofilm-Virus Interactions — **Knut Drescher**

**4:20 Paper 420c:** The Biophysics of Bacterial Biofilms Facilitate Surface Survival in Moving Fluids but May Reveal an Achilles Heel — **Paul Stoodley**

**4:45 Paper 420d:** Biofunctionalization of Implants through Thin Films — **Ellen Gawalt**

**5:10 Paper 420a:** Infection-Resisting Biomaterials — **Matthew Libera**

#### (421) Process Design: Conceptualization and Analysis of Chemical Processes I

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 409

Charles C. Solvason, Chair  
Emre Gençer, Co-Chair

**Sponsored by:** Systems and Process Design

**3:30 Paper 421a:** A General Framework for the Evaluation of Direct Nonoxidative Methane Conversion Strategies — **Kefeng Huang, James B. Miller, George W. Huber, James A. Dumesic, Christos T. Maravelias**

**3:49 Paper 421b:** Upstream Process Optimization to Reduce the Cost of Air Pollution Control — **Fred Hencken**

**4:08 Paper 421c:** Nonsmooth Simulation of Dry and Vaporless Tray Distillation Columns — **Suzane M. Cavalcanti, Paul I. Barton**

**4:27 Paper 421d:** Analysis of Chemical Process System Analysis with Entropy Generation — **John P. O'Connell**

**4:46 Paper 421e:** Effective Generalized Disjunctive Programming (GDP) Models for Modular Plant Design — **Qi Chen, Ignacio E. Grossmann**

**5:05 Paper 421f:** ProCAFD: A Computer-Aided Tool for Sustainable Process Synthesis, Design, Analysis and Improvement — **Anjan Kumar Tula, Mario Richard Eden, Venkat Venkatasubramanian, Rafiqul Gani**

**5:24 Paper 421g:** Systematic Process Design and Innovation Using Building Blocks — **Salih E. Demirel, Jianping Li, M. M. Faruque Hasan**

**5:43 Paper 421h:** Surrogate-Based Optimization for Biocatalytic Manufacturing of Diabetes Drug — **Chi-Hung Ho, Jieran Yi, Wei Sun, Xiaonan Wang**

#### (422) Process Intensification By Process Integration

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 335

Hanns Jörg Freund, Chair  
Honglin Qu, Co-Chair

**Sponsored by:** Process Intensification & Microprocess Engineering

**3:30 Paper 422a:** Intensifying Natural Gas Upgrading: Integrated Reactor Concepts for Syngas Production — **Götz Vesper**

**3:55 Break**

**4:20 Paper 422c:** Design Integration and Performance of Syngas Coolers and Steam System at the Kemper IGCC Power Plant — **Philip J. Keb, Xiaofeng Guan, Alan Hewitt, WanWang Peng, Guohai Liu, P. Vimalchand, Matthew Nelson, Tim Pinkston, Diane Revay Madden**

**4:45 Paper 422d:** Process Concept for Isolation of Low Molecular Weight Carboxylic Acids from Dilute Aqueous Feed — **Andreas Toth, Susanne Lux, Matthaeus Siebenhofer**

**5:10 Paper 422e:** Process Integration Using Block Superstructure — **Jianping Li, Salih E. Demirel, M. M. Faruque Hasan**

**5:35 Paper 422f:** Process Intensification Using Annular Centrifugal Extractor for Highly Exothermic Multi-Phase Di-Nitration Reaction — **Mrityunjay Sharma, Suneha Patil, Amol Kulkarni**

#### (423) Self and Directed Assembly at the Nanoscale II

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 311

Javen Weston, Chair  
Evan K. Wujcik, Co-Chair

**Sponsored by:** Nanoscale Science and Engineering Forum

**3:30 Paper 423a:** Investigating the Driving Forces of Assembly in Concentrated Electrolyte Solutions — **Arushi Prakash, Christopher Fu, Christopher J. Mundy, Jim Pfendtner**

**3:48 Paper 423b:** Chiro-magnetic Nanoparticles and Gels — **Jihyeon Yeom, Mahshid Chekini, Andre Moura, Nicholas Kotov**

**4:06 Paper 423c:** Effects of Matrix Chain Length on Miscibility of Nanoparticles — **Clement Koh, Sanat K. Kumar**

**4:24 Paper 423d:** Identifying Thermally and Kinetically Favorable Conditions for DNA-Mediated Assembly of Crystal Structures — **Runfang Mao, Jeetain Mittal**

**4:42 Paper 423e:** Origins of High-Pressure Structural Stability, Elasticity and Self-Healing Property in Ligand Capped Nanoparticles Supercrystals — **Tarak Patra, Subramanian Sankaranarayanan, Badri Narayanan**

**5:00 Paper 423f:** Generalized Nano-Thermodynamic Model for Predicting Size-Dependent Surface Segregation in Multi-Metal Alloy Nanoparticles from Smaller Particles — **Abhijit Chatterjee**

**5:18 Break**

**5:36 Paper 423h:** Controlled Self-Assembly of Cationic Polyelectrolytes and Anionic Surfactants in Microfluidic Channels — **Artem Bezrukov**

#### (424) Separation Processes in Biorefineries

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 324

Bandaru V. Ramarao, Chair  
Shri Ramaswamy, Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**3:30 Paper 424a:** Adsorption and Filtration of Lignocellulosic Hydrolyzates Using Fibrous Depth Filters — **Mary Jennifer Puthota, Thomas D. Stuart, Bandaru V. Ramarao**

**3:55 Paper 424b:** Process Modeling, Simulation and Optimization of Process Intensification in Integrated Biorefineries — **Huajiang Huang, Shri Ramaswamy**

**4:20 Paper 424c:** Process Intensification of the Hydrolysis of Cellulosic Fibers By Integration of Membrane Separations and Hydrolysis for Enzyme Recycle — **Venkata Jampana, Bandaru V. Ramarao**

**4:45 Paper 424d:** A Low Energy Separation Process to Isolate Xylose from Aqueous Hydrolyzate Streams — **Jagannadh Satyavolu**

**5:10 Paper 424e:** Multiobjective Optimization of Atpe Process for the 1,3PDO Production in a Palma Oil Biorefinery — **Camilo Monroy-Peña, Adriana Suesca Díaz, Gustavo Buitrago Hurtado, Carlos A. Martinez Riascos**

#### (425) Synthesis and Application of Inorganic Materials: Characterization

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 329

Xueyi Zhang, Chair  
Kumar Varoon Agrawal, Co-Chair

**Sponsored by:** Inorganic Materials

**3:30 Paper 425a:** Transient Modes of Zeolite Surface Growth: Establishing New Platforms for Catalyst Design from Mechanistic Understandings of Crystallization — **Madhuresh K. Choudhary, Manjesh Kumar, Rishabh Jain, Jeffrey D. Rimer**

**3:51 Paper 425b:** Microstructural Evolution of Self-Pillared Pentasil (SPP) Single-Unit-Cell Thick Siliceous Zeolite Under Steaming — **Yasmine Guefrachi, Michael Tsapatsis**

**4:12 Paper 425c:** Mesopore Differences between Pillared Lamellar MFI and MWW Zeolites — **Junyan Zhang, Dongxia Liu**

**4:33 Paper 425d:** Advanced Characterization of Hierarchical Zeolites for Optimal Xylene Separation — **I. C. Medeiros-Costa, C. Laroche, J. Perez-Pellitero, B. Coasne**

**4:54 Paper 425e:** Crystal Growth and Transformation of Gibbsite and Boehmite — **Xin Zhang, Jian Z. Hu, Carolyn Pearce, Katharine L. Page, Mark Bowden, Sue Clark, Kevin Rosso**

**5:15 Paper 425f:** Optimized Synthesis of Copper Oxide Nanoparticles Using a Simple Microwave-Assisted Method — **Shishir V Kumar, Adarsh Bafana, Prasad P Pawar, Si Amar Dahoumane, Clayton S Jeffries**

**5:36 Paper 425g:** Rheology of Pastes Based Zeolites — **Karla D. Guerrero G., Julio C. Vargas**

#### (426) Thermodynamics of Biomolecular Folding and Assembly

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 307

Sapna Sarupria, Chair  
Reid Van Lehn, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**3:30 Paper 426a:** Computational Investigation of the Effect of Backbone Chiral Inversions on Protein Folding — **Gul H. Zerze, Frank H. Stillinger, Pablo Debenedetti**



**3:45 Paper 426b:** The Hydrophobicity and Conformations of Common Glycosylation Motifs across the Kingdoms of Life — **Landon Mills, Gregg T. Beckham, Christina M. Payne**

**4:00 Paper 426c:** Simulation-Aided Design of Intrinsically Disordered Proteins with Tunable Phase Behavior — **Gregory L. Dignon, Jeetain Mittal, Wenwei Zheng**

**4:15 Paper 426d:** Towards a Thermodynamic Model for Predicting Coiled-Coil Protein Structures — **Mojtaba Jokar, Korosh Torabi**

**4:30 Paper 426e:** Molecular Simulations of a Biomimetic Polymer in Protein Aggregation — **Aviel Chaimovich, Christian Leitold, Christoph Dellago**

**4:45 Paper 426f:** Simulations and Experiments Delineate Amyloid Fibrilization By Peptides Derived from Glaucoma-Associated Myocilin — **Yiming Wang, Yuan Gao, Shannon E. Hill, Dustin J. E. Huard, Moya O. Tomlin, Raquel L. Lieberman, Anant K. Paravastu, Carol K. Hall**

**5:00 Paper 426g:** Inferring Effects of Sequence on Structure of Anti-Microbial Peptides through Molecular Dynamics and Normal Mode Analysis — **Faramarz Joodaki, Lenore M. Martin, Michael L. Greenfield**

**5:15 Paper 426h:** B-Wrapin Proteins Sequestering Amyloidogenic Proteins: Understanding Their Function and Designing Novel  $\beta$ -Wrapins with Improved Binding Affinities — **Asuka A. Orr, Sai Vamshi R. Jonnalagadda, Wolfgang Hoyer, Phanourios Tamamis**

**5:30 Paper 426i:** Driving Towards Selection of Folded and Highly Structured Nucleic Acid Templates — **Chiamaka Obianyor, Adriana Lozoya Colinas, Martha A. Grover, Nicholas Hud**

**5:45 Paper 426j:** Atomistic Simulation Studies of DNA-Porphyrin Nanoassemblies — **Lev Levintov, Harish Vashisth**

**(427) Thermophysical Properties: Mixtures and Complex Systems**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 305

Clare McCabe, Chair  
Erik E. Santiso, Co-Chair  
Sanket A. Deshmukh, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**3:30 Paper 427a:** A Simple Hard Convex Body Equation of State for Model Micelles in Water — **Arthur S. Gow, Laura Irwin, Nicholas Hart**

**3:49 Paper 427b:** Combining Molecular Simulations and Theory for Predicting the Binary Interaction Parameters of the NRTL Model — **Ashwin Ravichandran, Hla Tun, Rajesh Khare, Chau-Chyun Chen**

**4:08 Paper 427c:** Ring Additivity Group (RAG) Values for Thermochemical Properties of Unsubstituted Polycyclic Aromatic Hydrocarbons (PAH) Via Computational Chemistry — **Christopher Pope**

**4:27 Paper 427d:** Modeling the Solubilities of Binary Mixed Solids in Supercritical Carbon Dioxide — **Ricardo Macias-Salinas, Miguel Gonzalo Arenas-Quevedo, Octavio Elizalde-Solis**

**4:46 Paper 427e:** Separation Effects of Ethyl Lactate on Vapor-Liquid Equilibria of Acetone + Methanol Azeotropic System Using an Automatic Apparatus — **Hirofumi Matsuda, Rie Iizuka, Kiyofumi Kurihara, Katsumi Tochigi**

**5:05 Paper 427f:** Solubility of Lanosterol in Organic Solvents — **Li Ke, Daniel Forciniti**

**5:24 Paper 427g:** Prediction of Thermodynamic Properties, Structure and Vapour-Liquid Coexistence Properties of Levulinic Acid Using Monte Carlo Simulations — **Tamaghna Chakraborti, Anish Desouza, Jhumpa Adhikari**

**5:43 Paper 427h:** Thermal Conductivity of Several Alkanes Measured By Transient Hot-Wire Method — **Xueqiang Wang, Shuo Qiu, Jiangtao Wu**

**(428) The Use of CFD in Simulation of Multiphase Mixing Processes**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 334

Richard V. Calabrese, Chair  
Eric E. Janz, Co-Chair

**Sponsored by:** North American Mixing Forum

**3:30 Paper 428a:** Mixing and Turbulence in Gas-Liquid Systems: Bridging First Principle and Application Needs — **Emilio Baglietto, Thomas Eppinger, Simon Lo, Ravindra Aglave**

**4:00 Paper 428b:** Effect of Interfacial Forces on Mixing and Dispersion of Bubbles in Pipe Flows — **Mohsen Shiea, Antonio Buffo, Marco Vanni, Daniele Marchisio**

**4:30 Paper 428c:** CFD Modelling of Multi-Regime Multiphase Flows — **Simon Lo, Thomas Eppinger, Ravindra Aglave**

**5:00 Paper 428d:** Solid Suspension in Unbaffled Vessels Using Vertical Off-Center Agitators — **Dillon P. Moher, Kevin Myers, Eric E. Janz**

**5:30 Paper 428e:** Predictive Modeling for Particle Dissolution in Mixing Tanks — **Alexander Warning, Prasanna Venuvanalingam**

**(429) Tools for Product Design**  
**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, 319

Kenneth R. Cox, Chair  
Honglin Qu, Co-Chair  
Munish Sharma, Co-Chair

**Sponsored by:** Product Design

**3:30 Paper 429a:** The Properties of Gases and Liquids: 2020 — **J Richard Elliott, Thomas A. Knotts IV, W. Vincent Wilding, Kenneth Kroenlein**

**4:05 Paper 429b:** Computer-Aided Polymer Design Using COSMO-RS — **Nick Austin**

**4:28 Paper 429c:** Design of Electrosprayed Polysaccharides Nano/Microparticles for Drug and Vaccine Delivery — **Ngoc-Tram Le, Phong T. Huynh, James M. Myrick, Sitaraman Krishnan**

**4:51 Paper 429d:** QSAR Study of Combretastatin-like Chalcones As Cancer Cell Growth Inhibitors Using Linear and Non-Linear Machine Learning Approaches — **Shounak Datta, Mario Richard Eden**

**5:14 Paper 429e:** Integration of Heuristic Knowledge in a Skin-Care Emulsion Design — **Javier Arrieta-Escobar, Alvaro Orjuela, Fernando P. Bernardo, Mauricio Camargo, Laure Morel**

**5:37 Paper 429f:** Investigating Fluid-Particle Interactions in Expanded Beds Using CFD-DEM — **Victor Koppejan, Guilherme Ferreria, Haibin Wang, Dong-Qiang Lin, Marcel Ottens**

**(430) Topical Plenary: Advances in Fossil Energy R&D (Invited Talks)**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 321

Madhava Syamlal, Chair  
Chunshan Song, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**3:30 Paper 430a:** The U.S. Department of Energy's Fossil Energy Research and Development Priorities — **Steven Winberg**

**4:05 Paper 430b:** Low-Carbon Solution to Oil & Gas and Its Progress of Key Technologies — **Yuhan Sun**

**4:40 Paper 430c:** The Global Energy Challenge: What's Ahead — **Robert C. Armstrong**

**5:15 Paper 430d:** Advanced Modeling and Optimization for Future Generation Energy Systems — **Lorenz T. Biegler**

**(431) Tutorial on the Catalyst Cost Estimation Tool: Economic Insight for Catalyst Synthesis and Scale-up Research II (Invited Talks)**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 406

Joshua Schaidle, Chair  
Frederick Baddour, Co-Chair  
Kurt Van Aalsburg, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 431a:** Tutorial on the CatCost Tool: Microfluidic Nanoparticle Synthesis Example — **Kurt Van Aalsburg**

**4:10 Paper 431b:** Commercialization Example: Catalytic Indirect Liquefaction of Biomass — **Joshua A. Schaidle**



Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AIChEEvents app.



**(432) WIC 20th Anniversary: Celebrating Women in Chemical Engineering III (Invited Talks)**

**Tuesday, Oct 30, 3:30 PM**

David L. Lawrence Convention Center, Spirit of Pittsburgh A

Julianne L. Holloway, Chair  
Caryn L. Heldt, Co-Chair

**Sponsored by:** WIC 20th Anniversary: Celebrating Women in Chemical Engineering

**3:30 Session Introduction**

**3:33 Paper 432a:** Celebrating Women in Chemical Engineering: Past and Present — **Rosemarie D. Wesson**

**3:54 Paper 432b:** Engineered Models of the Gut-Brain Axis — **Abigail Koppes**

**4:15 Paper 432c:** Designer Nanoplexes for Delivery to Targeted Tissues — **Paula T. Hammond**

**4:36 Paper 432d:** Biomedical Applications of Emulsion Templating — **Elizabeth M. Cosgriff-Hernandez**

**4:57 Paper 432e:** AIChE's First Female Member – An Unsung Trailblazer of Chemical Engineering — **Christine Seymour**

**5:18 Paper 432f:** Silica Nanoparticles Act As Permeation Enhancers to Enable Oral Protein Delivery — **Kathryn A. Whitehead**

**5:39 Paper 432g:** The Role of Chemical Engineers in Pharmaceutical Development — **Sheena Reeves**

**(433) SBE's James E. Bailey Award Lecture**

**Tuesday, Oct 30, 6:00 PM**

Westin Convention Center, Allegheny Grand Ballroom I

Georges Belfort, Chair

**Sponsored by:** Awards Committee

**6:00 Paper 433a:** Turning Immunity On and Off — **Jeffrey A. Hubbell**

**(434) Ammonia Energy Technology Roadmap**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 318

Trevor Brown, Chair

**Sponsored by:** NH3 Energy+

**8:00 Paper 434a:** A Framework for Renewable Hydrogen and Ammonia Supply Chain Development — **Kaveh Rajab Khalilpour**

**8:15 Paper 434b:** Power-to-Ammonia-to-Power (P2A2P) for Local Electricity Storage in 2025 — **Kevin Hendrik Reindert Rouwenhorst**

**8:30 Paper 434c:** Cost Evaluation Study on CO<sub>2</sub>-Free Ammonia and Coal Co-Fired Power Generation Integrated with Cost of CCS — **Kazutaka Hiraoka, Yasushi Fujimura, Yoshiyuki Watanabe, Mototaka Kai, Ko Sakata, Yuki Ishimoto, Yuji Mizuno**

**8:45 Paper 542i:** Ammonia-Hydrogen Power for Combustion Engines — **Agustin Valera-Medina, Phil Bowen, Daniel Pugh**

**9:00 Paper 434e:** Ship Operation Using LPG and Ammonia As Fuel on Man B&W Dual Fuel ME-Lgip Engines — **René Sejer Laursen**

**9:15 Paper 434f:** Roadmap to All Electric Ammonia Plants — **John B. Hansen, Pat A. Han**

**(435) Additive Manufacturing of Energetics**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 413

Lori J. Groven, Chair  
Kyle T. Sullivan, Co-Chair

**Sponsored by:** Energetics

**8:00 Introductory Remarks**

**8:05 Paper 435a:** Solids Metrics for Successful 3D Printing of Energetic Feedstocks — **Brandon Ennis, Naseem Jibrin, Benjamin Ennis, Michael Winn, Bryan J. Ennis**

**8:30 Paper 435b:** 3D Printing of Metal-Polymer Composite Structures Via Fused Deposition Modeling — **Trevor Fleck, George Chiu, Emre Gunduz, Steven F. Son, Jeffrey Rhoads**

**8:50 Paper 435c:** Polymer Resin Systems for Precision Direct-Ink-Write Printing of Thermite-Loaded Inks — **Brian Howell, Eric Bukovsky, Paul Martinez, Matthew Durban, Michael Grapes, Alexandra Golobic, Kyle Sullivan, Alex E. Gash**

**9:10 Break**

**9:25 Paper 435d:** 3D Printing of Thermite Mixtures Using Static Mixing — **Michael Grapes, Elliot Wainwright, Matthew Durban, Kyle Sullivan, Alex E. Gash**

**9:45 Paper 435e:** Additive Manufacturing of Pyrotechnic Ignition Delays — **Ian Walters, Lori J. Groven**

**10:05 Paper 435f:** The Role of Particle Size on the Combustion of Boron Carbide/Sodium Periodate Biocidal Formulations — **Lance Kotter, Lori J. Groven**

**(436) Adsorption Applications for Sustainable Energy and Chemicals**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 311

Fateme Rezaei, Chair  
Armin D. Ebner, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**8:00 Paper 436a:** Competitive and Cooperative Adsorption of Ethanol on ZIF-8 in the Presence of 1-Butanol — **Benjamin Claessens, Ana Martin-Calvo, Nicolas Dubois, Julien Cousin-Saint-Remi, Joeri Denayer**

**8:18 Paper 436b:** Modeling of Multicomponent Sorption of Acetone-Butanol-Ethanol in a Fixed-Bed Adsorber Using the General Rate Model — **Haripriya Naidu, Alexander P. Mathews**

**8:36 Paper 436c:** Rare Earth Elements Extraction from Geothermal Brine Using Nanofluids — **Jian Liu, Michael Sinnwell, Paul Martin, Praveen K. Thallapally, B. Peter McGrail**

**8:54 Paper 436d:** Microporous Coating Modified 5A Zeolite for Propylene/Propane Separation — **Qiaobei Dong, Fanglei Zhou, Weiwei Xu, Huazheng Li, Syed Islam, Miao Yu**

**9:12 Paper 436e:** Development of MOF-74@Zeolite-5A Composite Adsorbents for H<sub>2</sub> Purification — **Qasim al-Naddaf, Harshul Thakkar, Ali Rownaghi, Fateme Rezaei**

**9:30 Paper 436f:** Microstructure Design of Carbon Materials and Matched Adsorption Process for the Low-Grade Methane Separation from Its Mixture with Nitrogen — **Kai Lu, Donglei Qu, Ying Yang, Ping Li, Jianguo Yu**

**9:48 Paper 436g:** Lithium Ion Sieves Vs. Li<sup>+</sup> Intercalation Electrodes As Effective and Energy-Efficient Materials for Li<sup>+</sup> Mining from Aqueous Resources — **Grace M. Nisola, Lawrence A. Limjuco, Chosel P. Lawagon, Khino J. Parohinog, Rey Eliseo C. Torrejos, Seong-Poong Lee, Wook-Jin Chung**

**10:06 Paper 436h:** Development of a Novel Emission Control Technology for Onshore-Offshore Applications — **Oluwatosin Oyelakin, Jeevan Dahal, Banchao Shu, Isaac Snyder, Priyanka Shahi**

**(437) Advances in Biocatalysis and Biosynthesis**

**Wednesday, Oct 31, 8:00 AM**

Westin Convention Center, Westmoreland West-Central

Jason T. Boock, Chair  
Nigel Reuel, Co-Chair

**Sponsored by:** Bioengineering

**8:00 Paper 437a:** Structural Insight into Enantioselective Inversion of an Alcohol Dehydrogenase Reveals a "Polar Gate" in Stereo-Recognition of Diaryl Ketones — **Ye Ni, Jieyu Zhou, Guochao Xu**

**8:18 Paper 437b:** Discovery of a Pathway for Halogenated, Terminal Alkene, and Terminal Alkyne Amino Acid Biosynthesis — **Jorge Marchand, Michelle C. Chang**

**8:36 Paper 437c:** De-Orphanizing the Nocardiosis-Associated Polyketide Synthase — **Kai Yuet, James Kuo, Chaitan Khosla**

**8:54 Paper 437d:** A Transcription Factor Decoy Strategy for Activation of *Streptomyces* Polyketide and Non-Ribosomal Peptide Gene Clusters — **Bin Wang, Fang Guo, Huimin Zhao**

**9:12 Paper 437e:** Yeast Intracellular Staining (yICS): Enabling Rapid Screening of High-Expressing Clones By Directly Quantifying Protein Expression at the Single-Cell Level — **Brett Hill, Syed Rizvi, Prabhu Ponnandy, Fei Wen**

**9:30 Paper 437f:** Discovery of Novel Genes Regulating Acyl-CoA Availability in *Yarrowia lipolytica* — **Difeng Gao, Michael Spagnuolo, Spencer Smith, Mark Blenner**

**9:48 Paper 437g:** A Rapid Cell-Free Approach to Production of Enzyme Biocatalysts and Their Encapsulation in Protective Virus-like Particles — **Bradley C. Bundy, Seung Ook Yang**

**(438) Advances in Bioseparations**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 301

Achyuta Teella, Chair  
Ketki Behere, Co-Chair

**Sponsored by:** Bio Separations

**8:00 Break**

**8:20 Paper 438b:** High-Throughput Process Development of Recombinant Human Serum Albumin Separation with Mixed-Mode Chromatography — **Wen-Ning Chu, Qi-Ci Wu, Shan-Jing Yao, Dong-Qiang Lin**

**8:40 Paper 438c:** Process Development of a Continuous Precipitation and Filtration Unit Operation for the Capture of Biotherapeutics — **Qin Gu, Zhao Li, Todd M. Przybycien, Andrew L. Zydney**

**9:00 Paper 438d:** Crystallisation of Short Peptides — **Wengian Chen, Xin Sian Chan, Mingxia Guo, Huaiyu Yang, Jerry Y.Y. Heng**

**9:20 Paper 438e:** Molecular Modeling to Efficiently Screen Chromatographic Separation of Challenging Enantiomer Separations — **Priyanka Oroskar Sharma, Pulak Sharma, Xiaoyu Wang, David W. House, Anil Oroskar, Asha Oroskar, Cynthia J. Jameson, Sohail Murad**

**9:40 Paper 438f:** Advances in Centrifugal Separation in Biotechnology — **Wallace Woon-Fong Leung**

**10:00 Paper 438g:** Separation of Intrinsically Magnetic Red Blood Cells Using Combination of Numerical Modelling and Microfluidic Magnetic Deposition System — **James Kim, Jeffrey J. Chalmers**

#### (439) Advances in Hydrogen and Syngas Production

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 321

Dushyant Shekhawat, Chair  
Daniel J. Haynes, Co-Chair  
Götz Vesper, Co-Chair  
Jianli Hu, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**8:00 Paper 439a:** High Purity Hydrogen Production in a 10 kWth Fixed Bed RESC Prototype System — **Sebastian Bock, Robert Zacharias, Viktor Hacker**

**8:21 Paper 439b:** High Purity Syngas and Hydrogen Coproduction from Natural Gas Using Cu-Fe Based Metal Oxides in a Chemical Looping System — **Sourabh Nadgouda, Mengqing Guo, Liang-Shih Fan**

**8:42 Paper 439c:** Process System Analysis of a High-Pressure Chemical Looping Based Hydrogen Production System — **Mandar Kathe, Frank Kong, Kate Clelland, Tyler Christeson, Andrew Tong, Liang-Shih Fan**

**9:03 Paper 439d:** Methane to Syngas by Chemical Looping Using FE-Ni Oxygen Carriers: Reactor Design and Process Modeling — **Hari C. Mantripragada, Goetz Vesper**

**9:24 Paper 439e:** Dry Reforming of Methane over Ni Based Lanthanum Zirconate Pyrochlore Catalysts: Deactivation Study — **Srikanth Bhattar, Swarom Kanihkar, Ashraf Abedin, Dushyant Shekhawat, Daniel J. Haynes, James J. Spivey**

**9:45 Paper 439f:** Pressure Dilution, a New Method to Prepare a Stable Ni/Fumed Silica Catalyst for the Dry Reforming of Methane to Produce Hydrogen — **Eduardo E. Wolf**

**10:06 Paper 439g:** A Novel Carbon-Resistant Perovskite Catalyst for Hydrogen Production Using Methane Dry Reforming — **Feraih Alenazey, Yousef Alyousef, Raja AL Otaibi, Adesina Adesoji A., Faisal Alotaibi, Bandar Alotaibi, Ghzzai Almutairi, Dai-Viet N. Vo**

#### (440) Advances in Industrial Modeling & Optimization: Methodologies, Tools and Applications

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 335

Yihui Tom Xu, Chair  
Raymond Wissinger, Co-Chair  
Hongbing (Raymond) Jian, Co-Chair

**Sponsored by:** Process Research and Innovation

**8:00 Paper 440a:** Comparison of First Principles and Parametric Models for the Design and Operation of a Spray Dryer for Whey Protein Production — **Anibal Barrios Quant, John Telotte, José Andrés Pérez Mendoza**

**8:18 Paper 440b:** Molecular Thermodynamic Model for Aqueous  $\text{Na}^+ - \text{K}^+ - \text{Mg}^{2+} - \text{Ca}^{2+} - \text{Cl}^- - \text{SO}_4^{2-}$  Quinary Electrolyte Systems — **Sheik Tanveer, Chau-Chyun Chen**

**8:36 Paper 440c:** Numerical Investigation of Heat Transfer in Fixed-Bed Reactors Filled with Complex Particle Shapes Using CFD — **Nico Jurtz, David Lucht, Matthias Kraume**

**8:54 Paper 440d:** Modeling of an Industrial Top-Fired Steam Methane Reformer — **Aaron Vandeputte, Awais Ahmed, Abdulaziz AL-Arifi, Adel Alghamdi, Ahmed AL-Khalaf**

**9:12 Paper 440e:** Modelling and Simulation of Industrial Purge Bins — **Charlotta Weber, Mohammad Al-haj Ali, Juha Visuri, Ville Alopaeus**

**9:30 Paper 440f:** Optimal Front-End Crude Scheduling for Refinery with Consideration of Proactive Unit Maintenance — **Honglin Qu, Qiang Xu**

**9:48 Paper 440g:** Thermodynamic Modeling of  $\text{CO}_2$  Absorption in Aqueous Amino Acid Salt Solutions with Symmetric Electrolyte NRTL Model — **Rajasi Shukre, Chau-Chyun Chen**

**10:06 Paper 440h:** Plantwide Process Design with Automatic Column Optimization, Sequencing and Stacking Using a Rigorous Process Simulator — **Yuan-Wei Ni, Jeffrey D. Ward**

#### (441) Advances in Optimization Under Uncertainty

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 409

Ruth Misener, Chair  
Fani Boukouvala, Co-Chair

**Sponsored by:** Computers in Operations and Information Processing

**8:00 Paper 441a:** A Sigmoidal Approximation for Chance-Constrained Nonlinear Programs — **Yankai Cao, Victor M. Zavala**

**8:19 Paper 441b:** A Global Optimization Algorithm for Nonconvex Chance-Constrained Programs with Continuous Random Variables — **Yuanxun Shao, Joseph Scott**

**8:38 Paper 441c:** On Solving Nonconvex Two-Stage Stochastic Programs with Generalized Benders Decomposition — **Can Li, Ignacio E. Grossmann**

**8:57 Paper 441d:** New Developments in Flexibility Analysis in the Framework of Design Space Definition — **M. Paz Ochoa, Carla Luciani, Stephen D. Stamatidis, Salvador García-Muñoz, Ignacio E. Grossmann**

**9:16 Paper 441e:** Adaptive Robust Optimization Under Uncertainty with Regret — **Chao Ning, Fengqi You**

**9:35 Paper 441f:** Hybrid Decision Rules in Multistage Adaptive Optimization — **Said Rahal, Zukui Li**

**9:54 Paper 441g:** An Algorithmic Cutting Plane Method for Solving Robust Optimization Problems with Endogenous Uncertainty — **Nikolaos Lappas, Anirudh Subramanyam, Chrysanthos E. Gounaris**

**10:13 Paper 441h:** Robust Explicit Optimization and Control within the Paroc Framework — **Nikolaos A. Dangelakis, Richard Oberdieck, Iosif S. Pappas, Efstratios N. Pistikopoulos**

#### (442) Atmospheric Chemistry and Physics I

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 319

Kristina Wagstrom, Chair  
Shunsuke Nakao, Co-Chair

**Sponsored by:** Air

**8:00 Paper 442a:** Measurement of Organic Aerosol Hygroscopicity and Oxidation Level As a Function of Volatility — **Kerrigan Cain, Eleni Karnezi, Spyros N. Pandis**

**8:20 Paper 442b:** Secondary Organic Aerosol Formation from Methylfurans By Nitrate Radical Oxidation — **Nga Lee Ng, Taekyu Joo, Masayuki Takeuchi, Matthew Alvarado**

**8:40 Paper 442c:** Polymorphism of Glutaric Acid Aerosols — **Phoebe Belser, Hemanta Timsina, Dabrina Dutcher, Timothy Raymond**

**9:00 Paper 442d:** Investigation of Levoglucosan Decay in Wood Smoke Smog-Chamber Experiments: The Importance of Aerosol Loading, Temperature, and Vapor Wall Losses in Interpreting Results — **Shunsuke Nakao, Jeffrey Pierce**

**9:20 Paper 442e:** CCN Activity and Particle Growth of Aging Diesel Exhaust Particles — **Humphrey Chukwuto, Frank Bowman**

**9:40 Paper 442f:** Elucidating the Effect of Photons and Aerosols on the Physical and Chemical Transformations of Atmospheric Mercury — **Sean Tacey, Lang Xu, Tibor Szilvási, James Schauer, Manos Mavrikakis**

#### (443) Best Practices in Pilot Plants

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 336

Rob Nunley, Chair  
Michael Trainor, Co-Chair

**Sponsored by:** Pilot Plants

**8:00 Paper 443a:** Optimal Design of Dynamic Experiments for Pilot Plants for  $\text{CO}_2$  Capture — **Anderson Soares Chinen, Joshua C. Morgan, Debansu Bhattacharyya, Benjamin P. Omell, Michael S. Matuszewski, David C. Miller**

**8:30 Paper 443b:** Review of the Different Type of Flow Elements and Technologies Suitable for Demo Scale Plants, Pilot Plants, and R&D Equipment with Installed Cost Comparison — **Leisl Dukhedini-Lalla**

**9:00 Paper 443c:** Innovating Chemical R&D Processes By Treating Them As Metaphorical “Chemical Processes” — **Darrell Velegol**

**9:30 Paper 443d:** Best Practices in Preventing Leaks in Pilot Plants, Laboratory Units, and Research Equipment — **Richard Palluzzi**

**(444) Biomolecules at Interfaces I**  
**Wednesday, Oct 31, 8:00 AM**  
Omni William Penn Hotel, Conference Center B

Susan Daniel, Chair  
Bernardo Yanez Soto, Co-Chair  
Amir M. Farnoud, Co-Chair

**Sponsored by:** Interfacial Phenomena

**8:00 Paper 444a:** Rhamnolipid Micellization and Adsorption Properties — **Yi Zhang, Tess Placek, Ruksana Jahan, Paschalis Alexandridis, Marina Tsiannou**

**8:15 Paper 444b:** Cholesterol Effects on Monolayer Phase Behavior, Morphology, and Surface Rheology — **Cain Valtierrez-Gaytan, Ian Williams, Steven Patton, Joseph A. Zasadzinski, Todd M. Squires**

**8:30 Paper 444c:** Effects of Curvature on the Lung Surfactant Monolayer — **Sourav Barman, Joseph A. Zasadzinski**

**8:45 Paper 444d:** Influence of Meibomian Lipids in Health and Disease on Tear Film Evaporation — **Daniela Blanco-Campoy, Rodrigo Velez-Cordero, Bernardo Yanez Soto**

**9:00 Paper 444e:** Effect of Entanglements in Lipid- and Polymer-Planar Membranes on Nucleation of Amyloid  $\beta$  and Its Fibril Growth Behavior — **Toshinori Shimanouchi, Miki Iwamura, Shintaro Deguchi, Saki Fukuma, Yukitaka Kimura**

**9:15 Paper 444f:** Physical Mechanism of Direct Permeation of Nanoparticle across Cell Membrane — **Hideya Nakamura, Kyohei Sezawa, Masataka Hata, Shuji Ohsaki, Satoru Watano**

**9:30 Paper 444g:** Effect of Membrane Fluctuation on Protein Adsorption to Lipid Membranes — **Saki Fukuma, Toshinori Shimanouchi, Yukitaka Kimura**

**9:45 Paper 444h:** Interaction of Small Molecules with Bacterial Outer Membrane Proteins — **Shikha Nangia**

**(445) Catalysis for C1 Chemistry I: Methanol Formation and Upgrading**  
**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center, 403

Pedro Serna, Chair  
Yunhai Bai, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 445a:**  $C_2$  Oxygenates from Syngas: Understanding and Improving Methanol Carbonylation Using Modified Mordenite Catalysts — **David Chester Upham, Marat Orazov, Thomas F. Jaramillo**

**8:18 Paper 445b:** Effects of Acid Site Proximity and Confinement in Zeolites on Methanol Dehydration Reaction Mechanisms Prevalent during Low-Temperature Catalysis — **John R. Di Iorio, Steven V. Nystrom Jr., Claire T. Nimlos, Alexander Hoffman, David Hibbitts, Rajamani Gounder**

**8:36 Paper 445c:** Deconvoluting the Competing Effects of Zeolite Framework Topology Versus Diffusion Path Length on Methanol-to-Hydrocarbon Reactions — **Yufeng Shen, Thuy T. Le, Donglong Fu, Joel E. Schmidt, Matthias Filez, Bert Weckhuysen, Jeffrey D. Rimer**

**8:54 Paper 445d:** Kinetic and Mechanistic Study of the Chemistry Involved in the Deactivation of Zeolite Catalysts during Methanol-to-Hydrocarbons Conversion — **Brandon Foley, Thomas Chen, Matthew Neurock, Aditya Bhan**

**9:12 Paper 445e:** Increasing Btp-X and C2-C3 Olefins in Methanol to Aromatics over Shape-Selective Zn-Si-HZSM-5 — **Abhay Zambare, Shi-Shang Jang, David Shan-Hill Wong, John OU**

**9:30 Paper 445f:** Mechanistic Details of Formic Acid Dehydration on  $TiO_2$  and  $ZrO_2$  Catalysts — **Stephanie Kwon, Ting Chun Lin, Enrique Iglesia**

**9:48 Paper 445g:** Highly Selective Conversion of Methanol to Propylene: Design of a MFI Zeolite with Selective-Blockage of (010) Surfaces — **Dali Cai**

**10:06 Paper 445h:** Selective Oxidation of Methane to Methanol: How to Live with the Selectivity-Conversion Limit — **Arvin Kakekhani, Allegra A. Latimer, Ambarish R. Kulkarni, Jens Nørskov**

**(446) Catalysis with Microporous and Mesoporous Materials I: Design and Synthesis of Materials**  
**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center, 404

Dongxia Liu, Chair  
Iman Noshadi, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 446a:** Organotemplate-Free Beta Zeolites: From Zeolite Synthesis to Hierarchical Structure Creation — **Ke Zhang, Sergio Fernandez, Michele L. Ostraat**

**8:20 Paper 446b:** Tuning the Molecular Design of Tertiary Amine Catalysts on Amorphous Mesoporous Silica Supports for Selective Glucose Isomerization and Acid-Base Cooperative Reactions — **Nicholas Brunelli, Nitish Deshpande, Takeshi Kobayashi, Chi-Ta Yang, Eun Hyun Cho, Mariah Whitaker, Aamena Parulkar, Marek Pruski, Li-Chiang Lin**

**8:40 Paper 446c:** Template Free Synthesis of Palladium Immobilized Ordered Mesoporous Resin for Drug Synthesis on a Chip — **Mahboubeh Nabavinia, Alexander Hesketh, Philip Wall, Elizabeth Kuhlman, Justin Ryan, Sabrina Rittweger, Matthew Knighton, Amanda Christon, Meagan Schweiger, Bridget Black, Alexis Lawless-Gattone, Iman Noshadi**

**9:00 Paper 446d:** Mesoporous Zeolites Produced By Solid Crystallization and Their Hydrogenation Properties — **Yuxin Wang, Cody Baxter, Yixin Liao, Shengnian Wang**

**9:20 Paper 446e:** Pillared Two-Dimensional Titanium Silicalite-1 Zeolite: Synthesis, Characterization and Catalytic Applications — **Wei Wu, Dongxia Liu**

**9:40 Paper 446f:** Synthesis Methods to Influence Framework Al Arrangements in CHA Zeolites and Consequences for  $NO_x$  Selective Catalytic Reduction — **John R. Di Iorio, Sichi Li, Subramanian Prasad, Ahmad Moini, William F. Schneider, Rajamani Gounder**

**10:00 Paper 446g:** Unraveling and Tuning Surface and Catalytic Chemistry of  $Zr_6O_8$  Nodes in Metal Organic Frameworks — **Dong Yang, Ruiping Wei, Guozhu Li, Qin Wu, Bruce C. Gates**

**(447) Cell Biomechanics, Adhesion and Migration I: Implications in Cancer**  
**Wednesday, Oct 31, 8:00 AM**  
Westin Convention Center, Butler

Ebong Eno, Chair  
Esther Gomez, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**8:00 Paper 447a:** Investigating the Spatiotemporal Dynamics of Paxillin Isoform Switching in Epithelial-Mesenchymal Transition — **Michael Reddick, Rajarshi Ghosh, Jan Liphardt**

**8:18 Paper 447b:** Breaking Away from the Pack: Lateral Compression Induces Single Cell Dissociation from Collectively Migrating Cancer Cells — **Robert Law, Zhizhan Gu, Bin Sheng Wong, Nianchao Wang, Konstantinos Konstantopoulos**

**8:36 Paper 447c:** Abnormal Nuclear Morphologies in Cancer: Role of Chromatin Regulators — **Andrew Tamashunas, Vincent J. Tocco Jr., James Matthews, Hendrik Luesch, Jonathan Licht, Richard Dickinson, Tanmay Lele**

**8:54 Paper 447d:** Identification of Nucleolin As a Novel L-Selectin Ligand Expressed on Head and Neck Squamous Carcinoma Cells — **Tove M. Goldson, Kevin L. Turner, Yinan Huang, Emily G. Caggiano, Susan M. Fennewald, Andres F. Oberhauser, Vicente A. Resto, Monica M. Burdick**

**9:12 Paper 447e:** Notch Signaling Inhibition Increases E-Selectin Ligand Activity and Alters Cell Migration of Mesenchymal-like Breast Cancer Cells — **Christian A. Showalter, Alexander O. Ostermann, Monica M. Burdick**

**9:30 Paper 447f:** Endothelial Glycocalyx Degradation in Disturbed Flow Enhances the Attachment of MCF7 Breast Cancer Cells Attachment to the Endothelium — **Alina Nersesyan, Solomon Mensah, Maeve Enright, Mark Niedre, Eno E. Ebong**

**9:48 Paper 447g:** Invited Speaker: Mechanisms of Metastatic Cell-Decision Making during Migration on Complex Microenvironments — **Cynthia Reinhart-King**



**(448) Computational Catalysis IV: Biomass Chemistry and Chemicals Production**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 402

Samir H. Mushrif, Chair  
Giannis Mpourmpakis, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 448a:** Mechanistic Study on C-C Coupling of Acetaldehyde on Partially Reduced CeO<sub>2-x</sub>(111)  
— *Chuanlin Zhao, Ye Xu*

**8:18 Paper 448b:** Transition Metal Oxides As Catalysts in the Diels-Alder Reaction between Furan and Methyl Acrylate — *Taha Salavati-fard, Efterpi Vasiliadou, Glen Jenness, Stavros Caratzoulas, Raul F. Lobo, Douglas J. Doren*

**8:36 Paper 448c:** Design of Solvent Composition for Acid-Catalyzed Reactions of Biomass-Derived Oxygenates Using Molecular Simulation-Derived Observables — *Alex Chew, Theodore Walker, Huixiang Li, Benginur Demir, Z. Conrad Zhang, George W. Huber, James Dumesic, Reid C. Van Lehn*

**8:54 Paper 448d:** Catalytic Hydrogenation of Carbon Monoxide to Formaldehyde in Functionalized Metal Organic Frameworks: An Investigation of Pathway and Uncertainty — *Lin Li, Sen Zhang, J. Karl Johnson*

**9:12 Paper 448e:** Theoretical Insights into Catalytic Upgrading of Ethanol over 2D MFI Zeolite — *Simuck F. Yuk, Junyan Zhang, Mal-Soon Lee, Sneha A. Akhade, Zhenglong Li, Vassiliki-Alexandra Glezakou, Roger Rousseau, Asanga B. Padmaperuma*

**9:30 Paper 448f:** Multicomponent Catalysis: Directing Reaction Pathways for Hydrodeoxygenation of Furfuryl Alcohol at Pd/TiO<sub>2</sub> Interfaces — *Shyam Deo, Michael J. Janik, J. Will Medlin, Eranda Nikolla*

**9:48 Paper 448g:** A DFT Study of the Support Effect on Hydrodeoxygenation Reaction — *Dan Huang, Matthew Young Cobllyn, Bavornpon Jansang, Nichaporn Sirimungkalakul, Thana Sornchamni, Goran N. Jovanovic, Liney Arnadottir*

**10:06 Paper 448h:** Homogeneous Catalysis of Ketene Production By Triethylphosphate — *Charles J. McGill, Sara Jo Taylor, Phillip R. Westmoreland*

**(449) Data-Driven Screening of Chemical and Materials Space**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 307

Poornima Padmanabhan, Chair  
Nav Nidhi Rajput, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**8:00 Paper 449a:** Connecting Experimental Conditions with Chemical Structure — *Eric Walker, Joshua Kammeraad, Jonathan Goetz, Ambuj Tewari, Paul M. Zimmerman*

**8:15 Paper 449b:** Symbolic Regression of Alpha Functions for Cubic Equations of State — *Marissa Engle, Nick Sahinidis*

**8:30 Paper 449c:** Predicting Hydrogen Storage in Half-a-Million MOFs Via Machine Learning — *Alauddin Ahmed, Donald J. Siegel*

**8:45 Paper 449d:** Inverse Design of Nanoporous Adsorbents for Gas Separation Applications — *Shachit S. Iyer, Ishan Bajaj, M. M. Faruque Hasan*

**9:00 Paper 449e:** From Atomistic to Systematic Coarse-Grained Models for Molecular Systems Using Path-Space Methods — *Vagelis A. Harmandaris, Evangelia Kalligiannaki*

**9:15 Paper 449f:** Classifying Antimicrobial and Multifunctional Peptides with Machine Learning — *Rainier Barrett, Andrew White*

**9:30 Paper 449g:** A Systematic Procedure for Designing Training Data for Molecular Property Prediction — *Bowen Li, Srinivas Rangarajan*

**9:45 Paper 449h:** Designing Proteins with Enhanced Antifreeze Activity Using Simulated Directed Evolution — *Daniel J. Kozuch*

**10:00 Paper 449j:** Transition State Geometry Prediction Using Neural Embeddings of Transition State Graphs — *Sai Krishna Sirumalla, Nathan Harms, Richard H. West*

**(450) Department Heads Forum (Invited Talks)**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 406

Valerie L. Young, Chair  
Edward J. Maginn, Co-Chair

**Sponsored by:** Department Heads Forum

**8:00 Paper 450a:** Transforming Undergraduate Chemical Engineering Education - a Report from NSF RED (Revolutionizing Engineering & Computer Science Departments) Projects — *Abhaya Datye, Jim Sweeney, Stephen Knisley*

**(451) Division Plenary: Materials Engineering & Sciences Division (Invited Talks)**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 327

John G. Ekerdt, Chair  
Yossef A. Elabd, Co-Chair

**Sponsored by:** Materials Engineering and Sciences Division

**8:00** MESD Poster Award Introductions

**8:05** Braskem Award Introduction

**8:10 Paper 451a:** Electrostatic Correlations in Polyelectrolyte Solutions — *Zhen-Gang Wang*

**8:40** Owens-Corning Award Introduction

**8:45 Paper 451b:** Harnessing Biomaterials to Study and Engineer Immune Function — *Christopher M. Jewell*

**9:15 Paper 451c:** Can Cells Do Calculus? Curvature and Edges As Cues for Structure Formation within Cells — *Kathleen J. Stebe*

**9:40 Paper 451d:** Strong Electrostatics Decouple Block Copolymer Morphology from Composition — *Sanat K. Kumar, Sebastian Russell, Luis Campos, Oleg Gang*

**10:05 Paper 451e:** The Challenges and Opportunities in Atomic Layer Etching of Functionally Enhanced Complex Materials — *Jane P. Chang*

**10:30** Concluding Remarks

**(452) Drug Delivery I: Biologics**

**Wednesday, Oct 31, 8:00 AM**

Westin Convention Center, Cambria

Rachel A. Letteri, Co-Chair  
Lorraine Leon, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**8:00 Paper 452a:** Polymersomes Deliver Active Enzyme to the Brains of Felines As Treatment of Neurodegeneration — *Jessica Kelly, Amanda Gross, Doug Martin, Mark E. Byrne*

**8:18 Paper 452b:** Poly(N-Isopropylacrylamide):Collagen Hydrogels for Tunable Syneresis and Drug Delivery — *Katarina DiLillo, Christopher Anderson*

**8:36 Paper 452c:** Erythrocytes As Carriers of Immunoglobulin Based Therapeutic Drugs — *Weihsang Ji, Richard Koepsel, Jill Andersen, Shelliza Carmali, Alan Russell*

**8:54 Paper 452d:** Mixed Posh Inhibitor Micelles As a Novel Leukemia Therapeutic Modality — *Josiah Smith, Leah Cardwell, David Porciani, Julie A. Nguyen, Andrea Nolla, Fabio Gallazzi, Donald Burke, Mark Daniels, Bret Ulery*

**9:12 Paper 452e:** Transcriptome Analysis of the Host Cell Response to Non-Viral Gene Therapy — *Matthew Tucker, Jacob Elmer*

**9:30 Paper 452f:** Investigating the Effect of Cross-Linker Branching and Conjugation Site on the Stability and Efficacy of Antibody-Drug Conjugates — *Joshua A. Walker, Francis Ledesma, Michelle R. Sorkin, Sneha R. Kabaria, Christopher A. Alabi*

**9:48 Paper 452g:** Invited Speaker: Lipid Nanoparticle Formulations for the Synergistic Co-Delivery of siRNA and mRNA — *Kathryn A. Whitehead*

**(453) Electrochemical Reactors, Fuel Cells, and Electrolyzers I**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 323

Al Sacco Jr., Chair  
Jamie Holladay, Co-Chair  
Michael Sees, Co-Chair

**Sponsored by:** Alternate Fuels and New Technology

**8:00** Welcoming Remarks

**8:05 Paper 453a:** NiMo-Ceria-Zirconia Anode for Direct Gasoline-Fed Solid Oxide Fuel Cells — *Su Ha, Xiaoxue (Christy) Hou, Kai Zhao, Qusay Bkour, M. Grant Norton*

**8:50 Paper 453b:** NiMo-Ceria-Zirconia Catalyst for Inert-Substrate-Supported Tubular Solid Oxide Fuel Cells Running on Model Gasoline — *Kai Zhao, Qusay Bkour, Grant Norton, Su Ha*

**9:20** Break

**9:50 Paper 453d:** Homogeneous Reaction Kinetics of Carbohydrates with Viologen Catalysts in Biofuel Cell Applications — *Hilary Bingham, Cassie Larimer, Meisam Bahari, John Harb, Randy S. Lewis*



**(454) Enabling Technologies for Immunotherapy Development**

**Wednesday, Oct 31, 8:00 AM**  
Westin Convention Center,  
Pennsylvania East

Arnab Mukherjee, Chair

**Sponsored by:** Immunotherapy

**8:00 Paper 454a:** Eradication of Primary and Cancer Stem Cells By Chemically Self-Assembled Nanoring Targeted T-Cells — **Carston R. Wagner**, Jacob R. Petersburg, Clifford M. Csiszar

**8:18 Paper 454b:** Inhibition of Peanut Induced Mast Cell Degranulation By Designing Covalent Heterobivalent Inhibitors — **Jaeho Shin**, Peter Deak, Baksun Kim, Amina Abdul Qayum, Girish Vitalpur, Kirsten Kloefer, Tanyel Kiziltepe, Mark Kaplan, Basar Bilgicer

**8:36 Paper 454c:** Remote Control of Engineered T Cells Using Photothermal Pulses — **Ian Miller**, Marielena Gamboa Castro, Lee-Kai Sun, Jason Weis, Gabriel Kwong

**8:54 Paper 454d:** Serum Antibody Profiling of Nivolumab/Azacytidine-Treated Acute Myeloid Leukemia Patients Via High-Throughput Sequencing of Peptide Phage-Display Library — **Jay R Adolacion**, Richard C. Willson, Navin Varadarajan

**9:12 Break**

**9:19 Paper 454e:** Yeast Surface Display Techniques Enhance Development of Chimeric Antigen Receptors for Hematologic Malignancies — **Lawrence A. Stern**, Laura Lim, Christian Huynh, Marissa M. Del Real, Lindsay O'Brien, Wen-Chung Chang, Michalina Silva, Brenda Aguilar, John C. Williams, L. Elizabeth Budde, Xiuli Wang, Christine E. Brown, Stephen J. Forman

**9:37 Paper 454f:** Efficient Incorporation of Matrix Protein M2 into Influenza Virus-like Particles (VLPs) for Improved Vaccine Manufacturing and Efficacy — **Andrew Zak**, Brett Hill, Syed Rizvi, Fei Wen

**9:55 Paper 454g:** Cytokine-like Regulation of T-Cell Fate Mediated By Tryptophan-Derived Microbiota Metabolites — **Arul Jayaraman**

**(455) Environmental Advances in Nuclear and Hazardous Waste Treatment**

**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center,  
320

Thong Hang, Chair  
Robert W. Peters, Co-Chair

**Sponsored by:** Solid and Hazardous Waste

**8:00 Paper 455a:** Effective Removal of Perchlorate from Groundwater By Bimetallic Porous Iron — **Dien Li**, Simona Murph, Dan Kaplan, Kathryn Taylor-Pashow, Fanny Coutelot, John Seaman, HyunShik Chang, Madan Tandukar

**8:30 Paper 455b:** Migrating High Performance Computing to the Amazon Cloud - Methods and Examples Using Environmental Systems Analysis — **Larry M. Deschaine**

**9:00 Paper 455e:** Design Optimization for Environmental Projects - A Primer on Optimization Methods — **Larry M. Deschaine**

**9:30 Paper 455c:** Quantifying Shifts in Trace Element Emissions from Coal-Fired Power Plants — **Daniel Gingerich**, Yifan Zhao, Meagan Mauter

**10:00 Paper 455d:** Adsorption of Cadmium, Nickel, and Lead on Modified Clinoptilolite: Equilibrium, Kinetic and Selectivity Studies — **Joshua Gorimbo**, Roick Chikati

**(456) Estimation and Control of Uncertain Systems**

**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center,  
408

Ali Mesbah, Chair  
Helen Durand, Co-Chair

**Sponsored by:** Systems and Process Control

**8:00 Paper 456a:** Estimating Uncertain Atmospheric Aerosol Dynamics with an Input Observer — **Dana L. McGuffin**, B. Erik Ydstie, Peter J. Adams

**8:19 Paper 456b:** Adaptive Model Predictive Control with Recursive Subspace Identification — **Iman Hajizadeh**, Mudassir Rashid, Ali Cinar

**8:38 Paper 456c:** Robust Model Predictive Control with Decomposed Disturbance Subsets for Less Conservative Control — **Tae Hoon Oh**, Jong Min Lee

**8:57 Paper 456d:** A Nonlinear Programming Framework for Estimating Spatial Coupling and Seasonal Transmission Parameters in Disease Transmission — **Todd Zhen**, Carl D. Laird

**9:16 Paper 456e:** Active Fault Diagnosis for Stochastic Linear Systems: Design Criteria and Implementation Issues — **Tor Aksel N. Heirung**, Ali Mesbah

**9:35 Paper 456f:** Stochastic Multiscale Model-Based Predictive Control Via Polynomial Chaos Theory: Manufacturing of Thin Films for Pharmaceutical Applications — **Jonggeol Na**, Jong Woo Kim, Kyeongsu Kim, Eranda Harinath, Mo Jiang, Jong Min Lee, Bernhardt L. Trout, Richard D. Braatz

**9:54 Paper 456g:** An Improved Set-Based State Estimation Method for Fault Detection and Diagnosis in Highly Nonlinear and Uncertain Chemical Processes — **Xuejiao Yang**, Joseph Scott

**10:13 Paper 456h:** Robust Model Based Control Via Closed-Loop Reference Trajectory Optimization — **Hao Li**, Christopher L. E. Swartz

**(457) Experimental, Theoretical, and Numerical Analysis of Transport Processes in Flow Reactors**

**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center,  
324

Haider Al-Rubaye, Chair

**Sponsored by:** Transport and Energy Processes

**8:00 Paper 457a:** Augmentation of the Rate of Mass Transfer Limited Liquid-Solid Heterogeneous Reactions by Turbulence Promoters — **Mohamad Elnaggar**

**8:25 Paper 457b:** Modeling and Experiments on the Effects of Increasing Flow Baffles on Dead Zone and Growth Performance of Microalgae in a Raceway Photobioreactor — **Matthew L. Alexander**, Chimezie Nwabugwu

**8:50 Paper 457c:** Implementation of a Flux-Dependent Anisotropic Diffusivity Model into Resolved-Particle CFD — **Behnam Partopour**, Anthony G. Dixon

**9:15 Paper 457d:** Experimental and Numerical Heat Transfer Investigation in a Mixing Vessel with Cooling Jacket — **Thomas Eppinger**, Alexander Heyter, Ravindra Aglave, Stefan Wollny

**9:40 Paper 457e:** Local Flow Regimes and Bubble Size Distributions in the Scrubbing-Cooling Chamber containing Dilute Fiber Suspensions of an Entrained-Flow Gasifier — **Xin Peng**, Yifei Wang, Zongyao Wei, Guangsu Yu, Fuchen Wang

**10:05 Paper 457f:** Chemical Mechanism and Kinetics of Cyclopentanone Combustion: A Theoretical and Rmg Approach — **Sarah Khanniche**, Matt Johnson, William H. Green

**(458) Forum Plenary: Sustainable Engineering Forum (Invited Talks)**

**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center,  
315

Ignasi Palou-Rivera, Chair  
Fengqi You, Co-Chair

**Sponsored by:** Sustainable Engineering Forum

**8:00 Paper 458a:** Research Challenges and Opportunities in Pathway Toward Sustainable Society — **Hamid Arastoopour**

**8:45 Paper 458b:** Innovative Methods for Teaching Sustainability Concepts in Engineering By Adopting 3D Printing, LCA and Computer Gaming into Undergraduate Curriculum — **Alexander Orlov**

**9:30 Paper 458c:** Prediction of Maximum Recoverable Mechanical Energy Via Work Integration: A Thermodynamic Modeling and Analysis Approach — **Aida Amini Rankouhi**, Yulun Huang

**9:50 Paper 458d:** Addressing Global Environmental Impacts Including Land Use Change in Life Cycle Optimization: Studies on Biofuels — **Daniel Garcia**, Fengqi You

**10:10 Paper 458e:** Incorporation of Safety and Sustainability in Conceptual Design Via a Return on Investment Metric — **Karen de Jesús Guillén-Cuevas**, Andrea Paulina Ortiz-Espinoza, Ecem Ozinan, Arturo Jiménez-Gutiérrez, Nikolaos Kazantzis, Mahmoud El-Halwagi



Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AIChEvents app.

**(459) Free Short Course - Redox Flow Batteries: From Fundamentals to Applications**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 306

Trung Van Nguyen, Chair

**Sponsored by:** Electrochemical Fundamentals

**8:00 Paper 459a:** Flow Batteries for Grid-Scale Energy Storage: A Historical Perspective, More Recent Approaches, and Specific Research Issues Addressed — **Robert F. Savinell**

**8:30 Paper 459b:** Materials and System Challenges in Flow Batteries for Large-Scale Energy Storage — **Trung Van Nguyen**

**9:00 Paper 459c:** Redox Flow Battery Technologies and Applications — **Wei Wang**

**9:30 Paper 459d:** Establishing Design Criteria for Cost-Effective Aqueous and Nonaqueous Redox Flow Batteries — **Fikile Brushett**

**(460) Hydrodynamics of Biological Systems**

**Wednesday, Oct 31, 8:00 AM**

Omni William Penn Hotel, Frick

Kelly M. Schultz, Chair

Amy M. Peterson, Co-Chair

**Sponsored by:** Fluid Mechanics

**8:00 Paper 460a:** Motility, Surface-Sensing and Signaling in Bacteria — **Pushkar Lele**

**8:30 Paper 460b:** Cross-Stream Distribution and Dynamics of Red Blood Cells in Sick Cell Disease — **Xiao Zhang, Michael D. Graham**

**8:45 Paper 460c:** Viscoelasticity, Thixotropy, and Wall Effects in Human Blood Rheology — **Jeffrey S. Horner, Antony N. Beris, Norman J. Wagner**

**9:00 Paper 460d:** Understanding Red Blood Cell Migration in Small Arterioles — **Amir Saadat, Qin M. Qi, Christopher Guido, Eric S. G. Shaqfeh**

**9:15 Paper 460e:** Determining the Role of Rheology in Human Mesenchymal Stem Cell Migration — **Maryam Daviran, Sarah M. Longwill, Jonah F. Casella, Kelly M. Schultz**

**9:30 Paper 460f:** CFD Simulations of Air-Particle Dynamics in Rabbit Airways — **Madhu V Majji, Taylor S. Geisler, Jana Kesavan, Eric S. G. Shaqfeh, Gianluca Iaccarino**

**9:45 Paper 460g:** Viscosity of Protein Solutions — **Eric M. Furst**

**10:00 Paper 460i:** Translational and Rotational Diffusion of Nanoparticles in Hyaluronic Acid Solutions — **Mythreyi Unni, Lorena Maldonado-Camargo, Shehaab Savliwala, Brittany Partain, Suresh Narayanan, Kyle Allen, Carlos Rinaldi**

**(461) Interfacial and Nonlinear Flows: Particle-Laden Systems**  
**Wednesday, Oct 31, 8:00 AM**  
**Omni William Penn Hotel, Phipps**

Hao Sun, Chair

Robert H. Davis, Co-Chair

**Sponsored by:** Fluid Mechanics

**8:00 Paper 461a:** Interfacial Failure of Polymer/Nanoparticle Interface and Its Influence to Flow Properties of Polymer Nanocomposites — **Shiwan Cheng**

**8:30 Paper 461b:** Rapid Particle Agglomeration Using Permeable Films — **Robert Davis, Alexander Zinchenko, Noemi Collado, Sydney Baysinger**

**8:45 Paper 461c:** Convection and Capillarity Induced Pattern Formation in the Spreading of a Concentrated Suspension of Rigid Spheres over a Liquid-Air Interface — **Rajesh Ranjan, Srishti Sehgal, Julia Kornfield, Arun Ramchandran**

**9:00 Paper 461d:** Pairwise Hydrodynamic Interaction between Two Squirmlers Pinned to a Fluid-Fluid Interface — **Nicholas G. Chisholm, Mehdi Molaei, Jiayi Deng, Robert L. Leheny, Kathleen J. Stebe**

**9:15 Paper 461e:** Bacterial Locomotion at Evolving Oil-Water Interface Prior to Elastic Film Formation — **Mehdi Molaei, Nicholas G. Chisholm, Jiayi Deng, Robert L. Leheny, Kathleen J. Stebe**

**9:30 Paper 461f:** Flow and Particle Dynamics on Interfaces with Non-Trivial Surface Rheology — **Harishankar Manikantan, Todd M. Squires**

**9:45 Paper 461g:** Simulation of Particle Deposition in an Evaporating Sessile Droplet — **Lihui Wang, Michael T. Harris**

**10:00 Paper 461h:** The Dynamics of Rising Oil-Coated Bubbles: Experiments and Simulations — **Songcheng Wang, Yi Zhang, J. Carson Meredith, Sven H. Behrens, Manoj Kumar Tripathi, Kirti Chandra Sahu**

**10:15 Paper 461i:** Electrokinetic Control of Viscous Fingering: From Theory to Experiment — **Tao Gao, Mohammad Mirzadeh, Martin Z. Bazant**

**(462) Ionic Liquids: Thermodynamics and Properties**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 316

Kevin N. West, Chair

Brooks D. Rabideau, Co-Chair

Xiangping Zhang, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**8:00 Paper 462a:** Ionicity and Hydrogen-Bonding As Critical Factors for Protic Ionic Liquids (PILs) Dissolution of Polysaccharides and Lignin — **Ezinne Achinivu**

**8:15 Break**

**8:30 Paper 462c:** How Proton Transfer Equilibria Influence Ionic Liquid Properties: Molecular Simulations of Alkylammonium Acetates — **Amir Taghavi Nasrabadi, Lev D. Gelb**

**8:45 Paper 462d:** Investigating Diffusivity of Solvated Ionic Liquids through Molecular Dynamics Screening — **Matt Thompson, Ray Matsumoto, Peter T. Cummings**

**9:00 Paper 462e:** Thermodynamics & Thermophysical Properties of Thermally Robust Ionic Liquids and Their Mixtures — **Kevin N. West, Benjamin Siu, Kelly Badilla, Alexander Badini, Brooks D. Rabideau, Mohammad Soltani, James H. Davis Jr.**

**9:15 Paper 462f:** Development of an Ionic Liquid Based Low-Temperature Electrolyte System for Sensing Applications of Planetary Exploration — **Yifei Xu, Wendy J. Lin, Marisa E. Gliege, Zuofeng Zhao, Hongyu Yu, Lenore L. Dai**

**9:30 Paper 462g:** Solubility and Diffusivity of Ammonia in Aprotic and Protic Ionic Liquids — **Tugba Turnaoglu, Mark B. Shiflett**

**9:45 Paper 462h:** Efficient and Reversible Separation of Ammonia with Ionic Liquid-Based Materials — **Shaojuan Zeng, Dawei Shang, Haifeng Dong, Xiangping Zhang, Suojiang Zhang**

**10:00 Paper 462i:** Electrical Conductivities of Binary and Ternary Deep Eutectic Solvents Via Molecular Simulation — **Braeden Federle, Kenneth M. Benjamin**

**10:15 Paper 462j:** Solvatochromic Evaluation of Hydrophobic Deep Eutectic Solvents — **Kyle McGaughy, M. Toufiq Reza**

**(463) Membrane-Based Organic Solvent Separations**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 303

Ryan Lively, Co-Chair

Andrew Livingston, Co-Chair

Geoffrey M. Geise, Co-Chair

**Sponsored by:** Membrane-Based Separations

**8:00 Break**

**8:18 Paper 463b:** Robust Polymeric Thin Film Composite Membranes for Organic Solvent Nanofiltration — **Ji Hoon Kim, Marcus Cook, Sang Hyun Park, Sun Ju Moon, Andrew G. Livingston, Young Moo Lee**

**8:36 Paper 463c:** Evidence for Entropic Selection of Xylene Isomers in Carbon Molecular Sieve Membranes — **Yao Ma, Ryan Lively**

**8:54 Paper 463d:** Design of Affinity and Size-Based Membranes for Organic Solvent Nanofiltration: Experiments and Simulations — **Lakshmeesha Upadhyaya, Xiaquan Sun, S. Ranil Wickramasinghe, Xianghong Qian**

**9:12 Paper 463e:** Polyethylene Glycol Grafting of Ultrafiltration Cross-Linked Polyimide Membranes Via Plasma Modification to Fabricate Organic Solvent Nanofiltration (OSN) Membranes — **Zhuo Fan Gao, Gui Min Shi, Yue Cui, Tai-Shung Chung**

**9:30 Paper 463f:** Membranes with Porous Organic Cages for Organic Solvent Nanofiltration — **Guanghui Zhu, Christopher W. Jones, Ryan Lively**

**9:48 Paper 463g:** Organic Solvent Nanofiltration Membranes Developed By Mussel-Inspired Strategy — **Lu Shao, Yanchao Xu Sr., Yanqiu Zhang**

**(464) Membrane Reactors**

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 304

Shamsuddin Ilias, Co-Chair

Theodore Tsotsis, Co-Chair

Dolly Chitta, Co-Chair

Seok-Jhin Kim, Co-Chair

**Sponsored by:** Membrane-Based Separations

**8:00 Paper 464a:** Cermet-Based Hydrogen Transport Membrane Reactors for Conversion of Methane to Value-Added Chemicals — **Dolly Chitta, Javier Alvarez, Camilo Corredor**

**8:20 Paper 464b:** Experimental and Numerical Study of an Intensified Water-Gas Shift (WGS) Reaction Process Using a Membrane Reactor (MR)/Adsorptive Reactor (AR) Sequence — *Huanhao Chen, Mingyuan Cao, Secgin Karagoz, Linghao Zhao, Vasilios Manousiouthakis, Theodore Tsotsis*

**8:40 Paper 464c:** Hydrogen Production in Pd-Based Membrane Reactor Via Reforming Reactions — *Simona Liguori, Jennifer Wilcox*

**9:00 Paper 464d:** Na-LTA Membranes with High Water Selectivity for Dimethyl Ether Production in a Catalytic Membrane Reactor — *Huazheng Li, Weiwei Xu, Qiaobei Dong, Fanglei Zhou, Syed Z. Islam, Surya Padinjarekutt, Miao Yu, Naomi Klinghoffer, Shiguang Li, Xinhua Liang*

**9:20 Paper 464e:** PDMS/Ceramic Composite Membrane in Glycerol Fermentation–PV Coupled Process for Biobutanol Production — *Haipeng Zhu, Jianwei Yuan, Tianpeng Chen, Fengxue Xin, Min Jiang, Gongping Liu, Wanqin Jin\**

**9:40 Paper 464f:** Thermochemical Stability of ZIF Membranes for Membrane Reactor Applications — *Seungju Lee, Jaesung Kim, Doohwan Lee*

**10:00 Paper 464g:** Enhancing CO<sub>2</sub>/CH<sub>4</sub> Separation Performance and Mechanical Strength of Mixed-Matrix Membrane Via Combined Use of Graphene Oxide and ZIF-8 — *Wen Li, Samarasinghe Arachchige Sulashi Chathushka Samarasinghe, Tae-Hyun Bae*

**(465) Metabolic and Process Engineering for Value-Added Products from Food Processing**  
**Wednesday, Oct 31, 8:00 AM**  
Westin Convention Center, Westmoreland East

Nuttha Thongchul, Chair  
Hesham EL Enshasy, Co-Chair  
Wenli Liu, Co-Chair

**Sponsored by:** Food

**8:00 Paper 465a:** Bioprocess Platform for High Cell Density Cultivation for Probiotic Yeast Production in Semi-Industrial Scale — *Hesham EL Enshasy, Mohamed Helmi Johari Masri, Amir Fuhaira Ishak, Mohd Shafiq Mohd Sueb, Roslinda Abd Malek, Siti Zulaiha Hanapi, Solleh Ramli, Ong Mei Leng, Ramlan Aziz*

**8:18 Paper 465b:** Glucose/Pachymaran Co-Feeding Enhanced Endo- $\beta$ -1,3-Glucanase Production By Trichoderma Harzianum Via Improving Cell Concentration and Maintaining Induction Effects — *Min-Jie Gao, Xiao-Bei Zhan*

**8:36 Paper 465c:** Phenotypic Adaptation of a Novel Bacterium for a Low-Cost Production of D-Lactic Acid — *Nuttha Thongchul, Sitanan Thitiprasert, Srettapat Limsampancharoen, Woraphot Toliang*

**8:54 Paper 465d:** Development of a Genome-Scale Metabolic Model for *S. Cerevisiae* to Facilitate Understanding of the Differences in Metabolism between Commercial Yeast Strains — *William T. Scott Jr., Ardric O. Arikal, Ayca Ozcan, David E. Block*

**9:12 Paper 465e:** Kinetics of Cell Growth and Invertase Production By the Biotherapeutic Yeast, *Saccharomyces Boulardii* — *Elsayed A Elsayed, Mohammad Wadaan, Hesham EL Enshasy*

**9:30 Paper 465f:** L-Lactate Production By a Potent Homofermentative *Bacillus* Sp. BC-001 — *Sitanan Thitiprasert, Kentaro Kodama, Somboon Tanasupawat, Phatthanon Prasitchoke, Budsabathip Prasirtsak, Tanapawarin Rampai, Vasana Tolieng, Jirabhorn Piluk, Suttichai Assabumrungrat, Nuttha Thongchul*

**9:48 Paper 465g:** (Keynote) Towards Efficient Bioproduction of Polymalic Acid and Malic Acid Production: System Metabolic and Process Engineering — *Xiang Zou*

**(466) Mixing Scale-up/Scale-down Issues in Pharmaceutical and Biopharmaceuticals Processes**  
**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center, 334

Piero M. Armenante, Chair  
Joerg Theuerkauf, Co-Chair

**Sponsored by:** North American Mixing Forum

**8:00 Paper 466a:** Hydrodynamics Characteristics of a Stirred Tank Provided with Angle-Mounted Impellers Using Computational and Experimental Approaches — *Chadakarn Sirasitthichoke, Ji Ma, Piero M. Armenante*

**8:30 Paper 466b:** Experimental and CFD Study of Mixing Two Fluids of Different Properties and Its Application in Biological Drug Product Manufacture — *Weixian Shi, Wei Chen, Rushikesh Patel, Christoph Bernoulli, Jasmine M. Rowe, Melissa Bentley, Nobel Vale, Dimuthu A. Jayawickrama*

**9:00 Paper 466c:** Recirculation Mixing and Heat Transfer Characteristics for Continuous Slug-Flow Cooling Crystallization — *Jingcai Cheng, Yan Zhang, Chao Yang, Mo Jiang, Zai-Sha Mao*

**9:30 Paper 466d:** Mini Continuous Stirred Tank Reactors (mini-CSTR) for Cell and Tissue Culture Applications — *Salvador Gallegos Martinez, Christian Carlos Mendoza Buenrostro, Pamela I. Rellstab-Sanchez, Ricardo Hernández Medina, Ingrid Anaya Morales, Mohamadmahdi Samandari, Everardo Gonzalez Gonzalez, Andrés García Rubio, Ciro Angel Rodríguez-González, Grissel Trujillo-de Santiago, Mario Moisés Alvarez*

**10:00 Paper 466e:** Power Dissipation and Power Numbers for a Retreat-Blade Impeller in Pharmaceutical Mixing Tanks and Reactors Using an Experimentally Validated Computational Approach — *Adam J. Bindas, Chadakarn Sirasitthichoke, Piero M. Armenante*

**(467) Modeling and Analysis of Chemical Reactors**  
**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center, 405

Anthony G. Dixon, Chair  
Sarah Feicht, Co-Chair  
Justin Federici, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 467a:** Oscillations and Hysteresis during Hydrocarbon Oxidation on a Diesel Oxidation Catalyst — *Oxford Peng, Michael Harold, Dan Luss*

**8:20 Paper 467b:** Large Eddy Simulations of Reaction Plumes and Micromixing — *John A. Thomas, Brian DeVincentis, Kevin Smith*

**8:40 Paper 467c:** Multi-Scale Modeling of an Annular Structured Catalytic Reactor for Steam Methane Reforming — *Florent Minette, Juray De Wilde*

**9:00 Paper 467d:** Ignition-Extinction Analysis of Methane Oxidative Coupling in Packed Bed Reactors — *Zhe Sun, David West, Vemuri Balakotaiah*

**9:20 Paper 467e:** Forced Periodic Reactor Operation with Simultaneous Modulation of Two Inputs: Nonlinear Frequency Response Analysis and Experimental Demonstration — *Matthias Felischak, Daliborka Nikolic, Menka Petkovska, Andreas Seidel-Morgenstern*

**9:40 Paper 467f:** Analysis of Flow Distribution and Reactions in a Closed Coupled Diesel Oxidation Catalyst — *Nishithan Balaji, Niket S. Kaisare, Preeti Aghalayam*

**10:00 Paper 544al:** Bifurcation Analysis of Coupled Homogeneous-Heterogeneous Reactions in Monoliths — *Bhaskar Sarkar, Balakotaiah Vemuri*

**(468) Modeling and Control of Crystallization**

**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center, 302

Meenesh R. Singh, Chair  
Christopher L. Burcham, Co-Chair

**Sponsored by:** Crystallization and Evaporation

**8:00** Introductory Remarks

**8:05 Paper 468a:** Identifying Nucleation and Growth Kernels of Crystallization — *Anish V. Dighe, James Fell, Meenesh R. Singh*

**8:25 Paper 468b:** A Novel Mode of Supersaturation Feedback Control: Semi-Batch Cooling Crystallization By Feeding Flow Rate Profiles — *Teng Zhang, Brigitta Nagy, Botond Szilagyi, Junbo Gong, Zoltan K. Nagy*

**8:45 Paper 468c:** Parameter Range Optimization and Modeling for a Reactive Crystallization Process — *Michael Dummeldinger, Daniel Treitler, Jose Tabora, Amanda Rogers*

**9:05 Paper 468d:** Enhanced Mass Transfer Process Control Via Hollow Fiber Membrane Assisted Antisolvent Crystallization — *Xiaobin Jiang, Linghan Tuo, Xuehua Ruan, Wu Xiao, Gaohong He*

**9:25 Paper 468e:** Experimental Implementation of a Model-Free Feedback Controller for the Size and Shape of Needle-like Crystals Growing in Suspension — *Ashwin Kumar Rajagopalan, Stefan Boetschi, Manfred Morari, Marco Mazzotti*

**9:45 Paper 468f:** Morphology Based Adsorption Kinetics of a Selectively Modulated Metal-Organic Framework — *Luke Huelsenbeck, Karl Westendorff, Gaurav Giri*



**10:05 Paper 468g:** Effects of Scale-up on the Mechanism and Kinetics of Crystal Nucleation — **René R. E. Steendam**, *Leila Keshavarz, Melian A. R. Blijlevens, Brian de Souza, Denise Croker, Patrick Frawley*

**10:25** Concluding Remarks

#### (469) Modeling of Lipid Membranes and Membrane Proteins

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 309

Shikha Nangia, Chair  
Reid Van Lehn, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**8:00 Paper 469a:** Nanoparticle Induced Rupture of Lipid Bilayers — **Sean Burgess**, *Aleksey Vishnyakov, Alexander Neimark*

**8:15 Paper 469b:** Nanoparticle Transport across Biomembranes: Probing the Limits and Consequences of Solubility-Diffusion Theories through Multiscale Modeling — **David J. Smith**, *L. Gary Leal, Samir Mitragotri, M. Scott Shell*

**8:30 Paper 469c:** Assembly of Charged Nanoparticles on Phase-Separated Lipid Bilayers — **Reid C. Van Lehn**

**8:45 Paper 469d:** Effect of Post-Translational Modification on the Self-Assembly of Membrane Proteins — **Shikha Nangia**

**9:00 Paper 469e:** Kir-Cholesterol Interactions: Molecular Simulations Reveal a Dynamic Ensemble of Lipid Ligands and a Composite Binding Domain of Asymmetric Concentration Dependence — **Nicolas Barbera**, *Manuela A.A. Ayee, Belinda S. Akpa, Irena Levitan*

**9:15 Paper 469f:** Characterizing Mechanisms for the Translocation of Charged Peptides across Lipid Bilayers with Enhanced Sampling Simulations — **Samarthaben J. Patel**, *Reid C. Van Lehn*

**9:30 Paper 469g:** Self-Assembly of Generic Scaffolding Proteins on Biologically Relevant Membranes — **Zack Jarin**, *Feng-Ching Tsai, Patricia Bassereau, Gregory A. Voth*

**9:45 Paper 469h:** Using Molecular Dynamics Simulations to Assess the Structure and Stability of Transmembrane Oligomeric Intermediates of Pore Forming Proteins — **Rajat Desikan**, *Amit Behera, Prabal K. Maiti, K. G. Ayappa*

**10:00 Paper 469i:** Scientific Benchmarks Guide Energy Function Improvements for Membrane Protein Modeling and Design — **Rebecca F. Alford**, *Patrick Fleming, Karen G. Fleming, Jeffrey J. Gray*

**10:15 Paper 469j:** Computational Modeling of Protein Interactions of the Matrix Domain of HIV-1 Gag — **Viviana Monje-Galvan**, *Alexander J. Pak, Gregory A. Voth*

#### (470) Multivariate Experimentation and Modeling for Pharmaceutical Products and Processes

**Wednesday, Oct 31, 8:00 AM**

Westin Convention Center, Fayette

Yuesheng Ye, Chair  
Nil Tandogan, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**8:00 Paper 470a:** Accelerating High-Throughput Experimentation with Templated Statistical Analysis — **Jacob Albrecht**, *Victor W. Rosso, Eric M. Saurer, Jose E. Tabora, Brendan C. Mack, Frederick Roberts, Grace Chiou, Jacob Janey*

**8:21 Paper 470b:** Process Fingerprinting Tools in the Development of an Alkylation Reaction — **Kevin Stone**, *Brian M. Wyratt, Emmanuel Adachi, Marguerite Mohan, Jonathan P. McMullen*

**8:42 Paper 470c:** Reactor Design for Continuous Synthesis of Pharmaceutical Intermediates: Correlation of Computational Fluid Dynamics and Design of Experiment Approaches — **Thomas D. Roper**, *Michael J. Bortner, Cameron Armstrong, Cailean Pritchard, Daniel Cook, Mariam Ibrahim, Bimbisar Desai, Yizheng Chen, Brian Marquardt, Patrick Whitham, Thouakesseh Zoueu*

**9:03 Paper 470d:** Optimal Design of Experiments for Building Fundamental Models of Pharmaceutical Production Processes — **Ali Shahmohammadi**, *Kimberley B. McAuley*

**9:24 Paper 470e:** Model-Based Design of Experiments for Pharmaceutical Reaction Development — **Kevin Stone**, *Jonathan P. McMullen, Dan Willard*

**9:45 Paper 470f:** Defining the Optimal Operating Window for Pharmaceutical Reactions Using the Dynamic Response Surface Methodology for All Measured Species — **Yachao Dong**, *Christos Georgakis, Jason Mustakis, Joel M. Hawkins, Jonathan P. McMullen, Shane T. Grosser*

**10:06 Paper 470g:** Sensitivity Analysis and Identification of Feasible Region of a Wet Granulation Continuous Pharmaceutical Manufacturing Process — **Nirupaplava Metta**, *Marianthi Ierapetritou, Rohit Ramachandran*

#### (471) Nanomaterials for Hydrogen Production and Fuel Cells I

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 412

Seung Soon Jang, Chair  
Doh Change Lee, Co-Chair

**Sponsored by:** Nanomaterials for Applications in Energy and Biology

**8:00 Paper 471a:** Molecular Engineering of Hydroxide Ion Conducting Aromatic Polymers and Their Applications in Alkaline Membrane Fuel Cells — **Chulsung Bae**

**8:25 Paper 471b:** Computational Design of Electrochemical CO<sub>2</sub> Reduction Catalysts — **Hyungjun Kim**

**8:50 Paper 471c:** Ni-Fe Alloy Nanowire Arrays As Outstanding Bifunctional Electrocatalysts for Overall Water Splitting — **Cheng-Ting Hsieh**, *Xui-Fang Chuah, Hao-Wei Lin, Shih-Yuan Lu*

**9:08 Paper 471d:** Rational Design of Single-Atom Electrocatalysts for Hydrogen Evolution Reaction — **Ara Cho**, *Suman Kalyan Sahoo, Jeong Woo Han*

**9:33 Paper 471e:** Nano-Structure Analysis of Catalyst Layer in Polymer Electrolyte Fuel Cell — **Shinichi Takahashi**, *Tomrau Ogawa, Hisashi Kashima, Norio Saito, Atsushi Ohma*

**9:51 Paper 471f:** Heterostructured Nanocatalysts for Electrochemical Energy Conversion Reactions — **Bing Joe Hwang**

**10:09 Paper 471g:** Metal Nanoparticle Surface Wetting and the Mitigation of Humidification Requirements for Proton Exchange Membrane Fuel Cells — **Anastasios Angelopoulos**, *Kevin Tonniss*

#### (472) Novel Nanoparticles and Nanostructured Materials for Catalysis

**Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 415

J. Ruud van Ommen, Chair  
Yomaira J. Pagan-Torres, Co-Chair

**Sponsored by:** Nanoparticles

**8:00 Paper 472a:** Hydrodechlorination of 1,2-Dichloroethane over Ag-Pd Catalysts Prepared By Controlled Surface Reactions — **Madelyn R Ball**, *Eric E. Stangland, Manos Mavrikakis, James A. Dumesic*

**8:20 Paper 472b:** Science of Shape-Controlled Synthesis of Metallic Nanoparticles — **Zhifeng Chen**, *Robert M. Rioux, Ji Woong Chang, Suprita Jharimune, Choumini Balasanthiran*

**8:40 Paper 472c:** Facile Novel Synthesis and Characterization of Gold-Copper Bimetallic Nanoclusters for Applications in Oxidation Catalysis — **Joseph Brindle**, *Michael M. Nigra*

**9:00 Paper 472d:** Atomic Layer Deposited Pt-Co Bimetallic Nanoparticles for Selective Hydrogenation — **Xiaofeng Wang**, *Yuzi Liu, Xinhua Liang*

**9:20 Paper 472e:** Facile Synthesis of 2D Molybdenum Carbide Nanosheets — **William P. Mounfield III**, *Yang Shao-Horn, Yuriy Román-Leshkov*

**9:40 Paper 472f:** Identification of Optimally Stable Nanoparticle Geometries Via Mathematical Optimization and Density-Functional Theory — **Natalie M. Isenberg**, *Zihao Yan, Michael G. Taylor, Christopher L. Hanselman, Giannis Mpourmpakis, Chrysanthos E. Gounaris*

**10:00 Paper 472g:** Niau Single Atom Alloys for the Oxidative Coupling of Methacrolein with Methanol — **Antonios Trimpalis**, *Georgios Giannakakis, Junjun Shan, Sufeng Cao, Maria Flytzani-Stephanopoulos, Zhen Qi, Juergen Biener*



Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AICHEvents app.



**(473) Panel: Pharmaceutical Engineering Challenges As Approached By Chemical Engineers Outside of Pharma (Invited Talks)**  
**Wednesday, Oct 31, 8:00 AM**  
 Westin Convention Center, Somerset

Jonathan McMullen, Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**8:00** Introductory Remarks

**8:10 Paper 473a:** Process Intensification Strategies in Chemical Synthesis: From Batch to Continuous Operation — **Kishori T. Deshpande**, Jianping Zeng, Ajit Vikram, Vivek Kumar, Utkarsh Ramesh, Karthik Balakrishnan, Nuri Oh, Trevor D. Ewers, Peter Trefonas III, Moonsub Shim, Paul J. A. Kenis

**8:37 Paper 473b:** Scaling Down a Purge Bin: A Multiscale Model-Centric Focus on Process Fundamentals — **Justin A. Federici**

**9:04 Paper 473c:** Energy Technology for a Carbon Constrained World Can It be Relevant for the Smaller Scale Chemical Processes — **Hugo S. Caram**

**9:31 Paper 473d:** Automated Continuous Crystallization and Mechanism Assessment of Zeolites — **Andrew Teixeira**

**9:58** Panel Discussion

**(474) Process Design: Conceptualization and Analysis of Chemical Processes II**

**Wednesday, Oct 31, 8:00 AM**  
 David L. Lawrence Convention Center, 410

Monica Zanfir, Chair  
 Ana I. Torres, Co-Chair  
 Apratim Bhattacharya, Co-Chair

**Sponsored by:** Systems and Process Design

**8:00 Paper 474a:** Dynamic Modeling of Phase Changes in Liquid-Liquid Mixtures — **Tobias Ploch**, Moll Glass, Andreas M. Bremen, Ralf Hannemann-Tamás, Alexander Mitsos

**8:19 Paper 474b:** From Graphical to Optimization-Based Distillation Column Design: A McCabe-Thiele-Inspired Math Program — **Lingxun Kong**, Christos T. Maravelias

**8:38 Paper 474c:** An MINLP Formulation for the Optimization of Heat-Pump Assisted Distillation Configurations — **Radhakrishna Tumbalam Gooty**, Tony Joseph Mathew, Mohit Tawarmalani, Rakesh Agrawal

**8:57 Paper 474d:** New Isotherm Model for S-Shaped Isotherm Data to be Used in Process Modeling and Its Model Reduction with Machine Learning Techniques — **Seongbin Ga**, Sangwon Lee, Jihan Kim, Jay H. Lee

**9:16** Break

**9:35 Paper 474f:** Heat Pump Assisted Configurations for Amine Based Natural Gas Sweetening Units — **Anoop Jagannath**, Ali Almansoori

**9:54 Paper 474g:** Conceptual Design and Exergy Analysis of the Cryogenic Energy Storage System Integrated with LNG Cold Utilization — **Inkyu Lee**, Il Moon

**10:13 Paper 474h:** Global Deterministic Surrogate-Based Process Design — **Artur M. Schweidtmann**, Wolfgang R. Huster, Alexander Mitsos

**(475) Reaction Engineering for Biomass Conversion I**

**Wednesday, Oct 31, 8:00 AM**  
 David L. Lawrence Convention Center, 401

Heather Mayes, Chair  
 M. Toufiq Reza, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 475a:** Oxidation of Lignin-Rich Residue from Deacetylation, Mechanical Refining, and Enzymatic Hydrolysis of Lignocellulose — **Jacob S. Kruger**, David Brandner, Camille Amador, Gregg T. Beckham

**8:21 Paper 475b:** Origins of Char during Fast-Hydropyrolysis of Biomass to Fuels — **Abhijit Talpade**, Richard Caulkins, Lan Xu, Yuan Jiang, Taufik Ridha, Nathan S. Mosier, Hilka Kentamaa, Rakesh Agrawal, W. Nicholas Delgass, Fabio H. Ribeiro

**8:42 Paper 475c:** Reaction Analysis and Kinetics of Propionic Acid Hydrodeoxygenation over Supported Pt and Ru Catalysis — **Joshua Gopeesingh**, Jesse Q. Bond

**9:03 Paper 475d:** Carbohydrate Stabilization Extends the Kinetic Limits of Chemical Polysaccharide Depolymerization — **Ydna M. Questell-Santiago**, Raquel Zambrano-Valera, Masoud Talebi Amiri, Jeremy S. Luterbacher

**9:24 Paper 475e:** Tuning Pathways for the Diversification of Biomass-Derived Coumalic Acid- Insights from First-Principles — **Ashwin Chemburkar**, Toni Plennig, Robert Johnson, Matthew Ryan, Aaron Rossini, Brent H. Shanks, Matthew Neurock

**9:45 Paper 475f:** Selective Catalytic Production of Polyols from Cellulose-Derived Levoglucosenone — **Siddarth H. Krishna**, Zachary R. Schmidt, James A. Dumesic, George W. Huber

**10:06 Paper 475g:** Kinetic Studies of Acid Hydrolysis of Linear Polysaccharides from Food Waste — **Elvis Ebikade**, Jonathan Lym, Basudeb Saha, Dionisios G. Vlachos

**(476) Recent Advances in Molecular Simulation Methods I**

**Wednesday, Oct 31, 8:00 AM**  
 David L. Lawrence Convention Center, 308

Harish Vashisth, Chair  
 Andrew White, Co-Chair  
 Erik E. Santiso, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**8:00 Paper 476a:** Predicting Virial Coefficients and Alchemical Transformations By Extrapolating Mayer-Sampling Monte Carlo Simulations — **Harold W. Hatch**, Sally Jiao, Nathan A. Mahynski, Marco A. Blanco, Vincent K. Shen

**8:15 Paper 476b:** First Principles Monte Carlo Simulations of Adsorption and Reaction Equilibria — **Evgenii Fetisov**, Mansi S. Shah, Michael Tsapatsis, J. Ilja Siepmann

**8:30 Paper 476c:** Molecular Exchange Monte Carlo: A Generalized Method for Identity Exchanges in Grand Canonical Monte Carlo Simulations — **Mohammad Barhaghi**, Korosh Torabi, Younes Nejahi, Loren Schwiebert, Jeffrey J. Potoff

**8:45 Paper 476d:** Computational Cluster-Integral Methods for Solutions — **Akshara Goyal**, Andrew J. Schultz, David A. Kofke

**9:00 Paper 476e:** Nucleus-Size Pinning for Determination of Nucleation Free-Energy Barriers and Nucleus Geometry — **Abhishek K. Sharma**, Fernando A. Escobedo

**9:15 Paper 476f:** A Free-Energy Diabat Approach to Polymorph Stability — **Kartik Kamat**, Baron Peters

**9:30 Paper 476g:** Free Energy Landscape with Experiment Directed Simulations and Enhanced Sampling — **Dilnoza Amirkulova**, Andrew White

**9:45 Paper 476h:** No More Histograms: Variational and Bayesian Approaches to Estimating Potentials of Mean Force — **Michael R. Shirts**, Andrew L. Ferguson

**10:00 Paper 476i:** Approaches to Finding Optimal Pathways and Flux Along Them in Multidimensional Free-Energy Hypersurfaces — **D. Ryan Barden**, Harish Vashisth

**10:15 Paper 476j:** Temperature Programmed Molecular Dynamics - Accessing Rare Events Using a Combination of Finite Time Sampling and Bias Potentials — **Abhijit Chatterjee**

**(477) Separation Processes and Waste Management**

**Wednesday, Oct 31, 8:00 AM**  
 David L. Lawrence Convention Center, 326

Jack D. Law, Chair

**Sponsored by:** Nuclear Engineering Division

**8:00 Paper 477a:** Direct Feed Low Activity Waste Test Platform - Alternative Demonstrations — **Reid Peterson**

**8:20 Paper 477b:** Improved Foam Control during High Level Radioactive Waste Processing — **Dan P. Lambert**, Wesley H. Woodham

**8:40 Paper 477c:** The Nature and Quantity of Solids Suspended in Hanford Nuclear Waste Supernatants — **Jacob G. Reynolds**, John Geeting

**9:00 Paper 477d:** Dechlorination of Electrorefiner Chloride Salt Via Ion-Exchange Using Ultra-Stable H-Y Zeolite — **Manish Wasnik**, Michael Simpson, Krista Carlson

**9:20 Paper 477e:** Iodine Adsorption in Reduced Ag<sub>2</sub> and Ag-Aerogel in Presence of Water and NO<sub>x</sub> — **Yue Nan**, Seungrag Choi, Abney Carter, Jisue Moon, Jiuxu Liu, Lawrence L. Tavlarides

**9:40 Paper 477f:** Kinetic Study of Ag Mordenite and Ag Functionalized Silica Aerogel Aging in Nuclear Fuel Reprocessing Off-Gases — **Seungrag Choi**, Yue Nan, Alexander Wiechert, Austin Ladshaw, Sotira Yiacoymi, Costas Tsouris, Lawrence L. Tavlarides

**10:00 Paper 477g:** Microflow Visualization of Tri-n-Butyl-Phosphate/ Dodecane and Nitric Acid in a Centrifugal Contactor — **Valmor F. de Almeida**, Joseph F. Birdwell Jr., David W. DePaoli, Costas Tsouris

**(478) Structured Adsorbents: Beyond Pellets and Beads****Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 305

Joeri Denayer, Chair

Roger D. Whitley, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**8:00 Paper 478a:** Synthesis and Characterization of UiO-66-NH<sub>2</sub> Metal-Organic Framework Cotton Composite Textiles — *Meagan A. Bunge, Kevin N. West, Christy Wheeler West, T. Grant Glover*

**8:20 Paper 478b:** Role of Bed Design Characteristics on the Effective Thermal Conductivity of a Structured Adsorbent — *Pravin B.C.A. Amalraj, Armin D. Ebner, James A. Ritter*

**8:40 Paper 478c:** Development of 3D-Printed Polymer-Zeolite Composite Monoliths for Gas Separation — *Harshul Thakkar, Shane Lawson, Ali Rownaghi, Fateme Rezaei*

**9:00 Paper 478d:** Emulsion Templated Polymers As Supports for Metal Organic Frameworks — *Jacob I. Deneff, Krista S. Walton*

**9:20 Paper 478e:** UTSA-16 Growth within 3D-Printed Co-Kaolin Monolith with High Selectivity for CO<sub>2</sub>/CH<sub>4</sub>, CO<sub>2</sub>/N<sub>2</sub>, and CO<sub>2</sub>/H<sub>2</sub> Separation — *Shane Lawson, Marc St. Amour, Fateme Rezaei, Ali A. Rownaghi*

**9:40 Paper 478f:** Fibrous Carbon Molecular Sieve with 3-5 Å Tunable Pores for Many Industrial Gas Separations — *Jay (Junqiang) Liu, Janet Goss, Rob Golombeski, Ted Calverley*

**10:00 Paper 478g:** HETP Analysis of Structured Adsorbents for Gas Separation Processes — *Roberto Mennitto, Ishan Sharma, Daniel Friedrich, Stefano Brandani*

**(479) Teaching Communication Skills to Engineers (Written, Oral, Data Visualization)****Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 411

Shannon Ciston, Chair

Katie Cadwell, Co-Chair

Christy Wheeler West, Co-Chair

**Sponsored by:** Undergraduate Education

**8:00 Paper 479a:** Ready, Set, Speak! Classroom Activities for Developing Oral Communication Skills — *Elif E. Miskioğlu*

**8:18 Paper 479b:** Know Your Audience: Expanding the Range of Scientific Communication in the Classroom — *Sarah A. Wilson*

**8:36 Paper 479c:** The Art of Communication: Ways to Incorporate Active Learning to Develop Student Communication — *Alex J. Bertuccio*

**8:54 Paper 479d:** The Technical Memo — *Valerie L. Young, Michael E. Prudich, Darin Ridgway, Douglas J. Goetz*

**9:12 Paper 479e:** Starting Early and Small with Technical Communication: Sophomores, Plots, and Captions — *Christy Wheeler West*

**9:30 Paper 479f:** Technical Communications Emphasis in Senior Chemical Engineering Laboratory Course — *Marjorie S. Went, Shannon Ciston*

**9:48 Paper 479g:** Teaching Technical Communication to Chemical Engineering Undergraduate Students through the Use of a Learning Community and Linked Courses — *Stephanie Loveland, Michael Satterwhite*

**10:06 Paper 479h:** Adapting the COPE (Clarity, Organization, Precision, and Economy) Framework As a Writing Guide and Assessment Framework — *Kevin Hadley, King Adkins*

**(480) Transport of Particulate Solids (Mechanical, Pneumatic and Hydraulic Conveying/Slurry)****Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 414

Stefan Radl, Chair

Gary Liu, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**8:00 Paper 480a:** Why and How to Select and Design a Dense Phase Conveying System? — *Gary Liu*

**8:18 Paper 480b:** Assessment of Effects of Flow Enhancers in Pneumatic Conveying of Cohesive Dairy Powders: CFD-DEM Simulation — *Akeem Olaleye, Orest Shardt, Gavin Walker, Harry E.A. Van den Akker*

**8:36 Paper 480c:** Towards Understanding Fly Ash Transport and Deposition in the Human Respiratory System: Effects of Physiological Conditions and Fly Ash Properties — *Siming You, Zhiyi Yao, Ruiqi Fu, Chi-Hwa Wang*

**8:54 Paper 480d:** Large Eddy Simulation of Particle Laden Flows — *John A. Thomas, Kevin Smith, Brian DeVincentis*

**9:12 Paper 480e:** Strandphase®: The Gentle Pneumatic Conveying Solution — *Amit K. Gautam, William F. Sahrhage III, Joseph Lutz*

**(481) Tribute to Jacques L. Zakin: Scholar, Teacher and Mentor I (Invited Talks)****Wednesday, Oct 31, 8:00 AM**

Omni William Penn Hotel, Conference Center A

Stuart L. Cooper, Chair

Umit S. Ozkan, Co-Chair

**Sponsored by:** Interfacial Phenomena

**8:00 Paper 481a:** A Tribute to Jack Zakin: A Brief Introduction — *Umit S. Ozkan*

**8:10 Paper 481b:** Rheological Complexity in Yield-Stress Fluids — *Morton Denn, Daniel Bonn*

**8:40 Paper 481c:** Drag Reduction in Dilute Gas-Solids Suspension Flow in Tubes—Revisited — *Robert Pfeffer*

**9:10 Paper 481d:** Nanostructural Aspects of Drag-reduction — *Yeshayahu (Ishij) Talmon*

**9:40 Paper 481e:** Context of Jacques L. Zakin's Contributions to our Understanding of Drag Reduction — *Kurt W. Koelling*

**10:10 Paper 481f:** Heat Transfer Enhancement in Turbulent Drag Reducing Surfactant Solutions — *Andrew Maxson*

**(482) USA-China Progress in Biomass Conversion Technologies I****Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 325

Shijie Liu, Chair

Zhongyang Luo, Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**8:00 Paper 482a:** Rapid and Low Temperature (< 80 °C) Hydrotrope Chemistry for Economic and Sustainable Production of Sugar/Biofuels, and Lignocellulosic Nanomaterials — *J.Y. Zhu*

**8:22 Paper 482b:** HPLC/Qtof-MS for Analysis of Oligomeric Compounds (pyrolytic lignin) from Crude Bio-Oils and Products from Pyrolysis of Model Compounds — *Simin Li, Wenbo Wang, Kongyu Lu, Yi Yang, Zhongyang Luo*

**8:44 Break**

**9:06 Paper 482d:** Steam Reforming of Toluene and Biomass Tar over Biochar Supported Ni Nanoparticles: Effects of Ni Particle Size on Catalytic Activity and Stability — *Zhenyi Du*

**9:28 Paper 482e:** Optimize Fermentation Conditions By Using Glucose As a Substrate to Produce (R)-3-Hydroxybutyric Acid with *Burkholderia Cepacia* — *Guoyu Dong, Shijie Liu*

**9:50 Paper 482f:** Organosolv Pretreatment of Hybrid Pennisetum for the Production of Lignin and Enzymatically Digestible Cellulose — *Xinshu Zhuang, Xuesong Tan, Wen Wang, Qiang Yu, Wei Qi, Qiong Wang, Zhenhong Yuan*

**(483) Young Faculty Forum (Invited Talks)****Wednesday, Oct 31, 8:00 AM**

David L. Lawrence Convention Center, 407

Anju Gupta, Chair

Aravind Suresh, Co-Chair

**Sponsored by:** Young Faculty Forum

**8:00 Paper 483b:** Lessons Learned during the Tenure-Track Process — *Placidus B. Amama*

**8:20 Paper 483a:** Ten Hints for Better Teaching — *Phillip C. Wankat*

**(484) Area Plenary: Carbon Nanomaterials (Invited Talks)****Wednesday, Oct 31, 8:30 AM**

David L. Lawrence Convention Center, 310

Anson Ma, Chair

Geyou Ao, Co-Chair

**Sponsored by:** Carbon Nanomaterials

**8:30 Paper 484a:** Chemical Engineering Science for Graphene Technology Development — *Robert H. Hurt*

**9:30 Paper 484b:** From Energy Harvesting to Living Plants - Concepts in Biosensing and Energy Conversion Using Carbon Nanomaterials — *Michael Strano*

**(485) Ammonia Fuel and Energy Storage: Cracking & Fuel Cells****Wednesday, Oct 31, 9:45 AM**

David L. Lawrence Convention Center, 317

Trevor Brown, Chair

**Sponsored by:** NH<sub>3</sub> Energy+

**9:45 Paper 485a:** Ammonia As a Hydrogen Carrier for PEM Fuel Cells — *Yoshitsugu Kojima*

**10:00 Paper 485b:** Catalytic Membrane Reactors for Efficient Delivery of High Purity Hydrogen from Ammonia Decomposition — **Zhenyu Zhang**, *Simona Liguori, J. Douglas Way, Colin A. Wolden*

**10:15 Paper 485c:** Development of a Highly Efficient CO<sub>x</sub>-Free Ammonia Dehydrogenation System for Fuel Cell Applications — **Young Suk Jo**, *Junyoung Cha, Hyuntae Sohn, Suk Woo Nam, Chang Won Yoon*

**10:30 Paper 485d:** Material Discovery and High Throughput Exploration of Ru Based Catalysts for Low Temperature Ammonia Decomposition — **Katie McCullough**, *Travis Williams, Benjamin Ruiz, Jochen Lauterbach*

**10:45 Paper 485e:** Functionalized Ordered Mesoporous Silica Composites As Potential Ammonia Storage Materials — **Zhu Ming**, *Pan Xingxiang, Mei Hua*

**11:00 Paper 485f:** Development of Catalytic Reactors and Solid Oxide Fuel Cells Systems for Utilization of Ammonia — **Koichi Eguchi**, *Yosuke Takahashi, Takahiro Matsuo, Hayahide Yamasaki, Hidehito Kubo, Akihiro Okabe, Takenori Isomura*

#### **(486) Sustainable Ammonia Synthesis: Better & Beyond Haber-Bosch**

**Wednesday, Oct 31, 9:45 AM**  
David L. Lawrence Convention Center, 318

Trevor Brown, Chair

**Sponsored by:** NH3 Energy+

**9:45 Paper 486a:** Importance of Reaction Mechanism Involved in Design of the Catalyst and the Reactor for Future Ammonia Synthesis — **Ken-ichi Aika**

**10:00 Paper 486b:** Ammonia Absorption and Desorption in Ammines — **E L Cussler**

**10:15 Paper 486c:** Scale up and Scale Down Issues of Renewable Ammonia Plants: Towards Modular Design — **Antonio Sánchez**, *Mariano Martin*

**10:21 Paper 486d:** Advances in Making High Purity Nitrogen for Small Scale Ammonia Generation — **David Toyne**, *Jay Schmucke*

**10:27 Paper 486e:** Early Transition Metal Carbides and Nitrides for Sustainable Ammonia Synthesis — **Zixuan Wang**, *Levi T. Thompson*

**10:33 Paper 486f:** Advanced Catalysts Development for Small, Distributed, Clean Haber-Bosch Reactors — **Adam Welch**, *Jonathan Kintner, Jason Ganley, Christopher Cadigan, Ryan O'Hayre, Joseph Beach*

**10:39 Question & Answer Session:** Better Haber-Bosch

**10:45 Paper 486g:** Ammonia Synthesis Via Radiofrequency Plasma Catalysis — **Javishk Shah**, *Weizong Wang, Annemie Bogaerts, Maria Carreon*

**10:51 Paper 486h:** Terrestrial Energy, National Lab, Southern Company – Partnership Overview Using Integral Molten Salt Reactor Technology with Hys Acid for Hydrogen Production — **John Kutsch**

**10:57 Paper 486i:** Creating a Redox Materials Database for Solar-Thermochemical Air Separation and Fuels Production — **Josua Vieten**, *Patrick Huck, Dorothy Guban, Matthew Horton, Brendan Bulfin, Martin Roeb, Kristin Persson, Christian Sattler*

**11:03 Paper 486j:** Microwave Catalysis for Ammonia Synthesis Under Mild Reaction Conditions — **Jianli Hu**, *Hanjing Tian, Yan Luo, Xinwei Bai, Dushyant Shekhawat, Christina Wildfire, Victor Abdelsayed, Michael J. Spencer, Robert A. Dagle, Stephen Davidson, Albert E. Stiegman*

**11:09 Question & Answer session:** Beyond Haber-Bosch

#### **(487) John M. Prausnitz AIChE Institute Lecture**

**Wednesday, Oct 31, 11:15 AM**  
David L. Lawrence Convention Center, Spirit of Pittsburgh A

J. Karl Johnson, Chair

**Sponsored by:** Awards Committee

**11:15 Paper 487a:** Accelerating Development and Intensification of Chemical Processes — **Klavs F. Jensen**

#### **(488) 2D Nanocomposites: New Composites with 2-Dimensional Nanomaterials**

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 329

Pingwei Liu, Chair  
Evan K. Wujcik, Co-Chair  
Vilas G. Pol, Co-Chair  
Yang Lu, Co-Chair

**Sponsored by:** Composites

**12:30 Paper 488a:** Dry Solid Lubricant Comprising 2D Materials — **Farshid Sadeghi**, *Vilas G. Pol, Abdullah Alazemi*

**12:55 Paper 488b:** Graphene/Montmorillonite Coating As a Lightning Strike Protective Layer for Epoxy-Based Composites: Thermal Analysis By Molecular Dynamics Simulation — **Farzin Rahmani**, *Sasan Nouranian*

**1:12 Paper 488c:** Improved Antibacterial Properties of a Silver-Based Metal Organic Framework through Its Decoration with Graphene Oxide — **Ahmad Arabi Shamsabadi**, *Mostafa Dadashi Firouzjaei, Mohammad Sharifian Gh., Ahmad Rahimpour, Masoud Soroush*

**1:29 Break**

**1:46 Paper 488e:** Plasmons Increase Catalytic Reduction By Metal Nanoparticles Reduced on Monolayer Transition Metal Dichalcogenide — **D. Keith Roper**, *Ricardo Romo, Alexander O'Brien*

**2:03 Paper 488f:** Composite Nanomaterials for 3rd Generation Solar Cells — **Wei Wei**

**2:20 Paper 488g:** Nature-Derived Nanocomposite for the Supercapacitors and Lithium-Ion Batteries — **Mengyao Gao**, *Yan-Cheng Lin, Chien-Chung Shih, Wen-Chang Chen*

**2:37 Paper 488h:** Controlled Synthesis of Graphene By Chemical Vapour Deposition — **Zhengtang Luo**, *Yao Ding, Ruizhe Wu, Irfan Haider Abidi*

#### **(489) ABET Updates and Insights (Invited Talks)**

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 407

Randy S. Lewis, Chair  
Douglas Ludlow, Co-Chair

**Sponsored by:** Undergraduate Education

**12:30 Paper 489a:** Education and Accreditation Committee Discusses Updates and Insights Regarding ABET Accreditation — **Randy S. Lewis**, *Douglas K. Ludlow*

#### **(490) Advanced Fuel Cell, Hydrogen Generation & Storage Technologies**

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 324

Julie N. Renner, Chair  
Maureen H. Tang, Co-Chair

**Sponsored by:** Transport and Energy Processes

**12:30 Paper 490a:** Integration Options of Electrochemical Hydrogen Pumping — **Michael Bampaou**, *Kyriakos Panopoulos, Athanasios I Papadopoulos, Panos Seferlis, S. S. Voutetakis*

**12:50 Paper 490b:** Advanced Water Management in Polymer Electrolyte Fuel Cells Using Engineered Gas Diffusion Layers with Patterned Wettability — **Antoni Forner-Cuenca**, *Victoria Manzi-Orezzoli, Lorenz Gubler, Thomas J. Schmidt, Pierre Boillat*

**1:10 Paper 490c:** Theoretical Observations of Hydrogen Trapping and Hydrogen-Induced Failure in Pd-Based Alloys — **Peter C. Psarras**, *Jennifer Wilcox*

**1:30 Paper 490d:** In-Situ Fluorescence Spectroscopy Study of the Chemical Degradation and Mitigation of the Radiation Induced Grafted Fep Based Pems — **Xue Li**, *Yunzhu Zhang, Yang Zhao, Xiaofeng Xie, Vijay Ramani*

**1:50 Paper 490e:** Dual Set-Point Cascade Control for Water Management in Methanol Fuel Cells — **Oscar Crisalle**, *Zuhair Alyousef, Shyam Mudiraj*

**2:10 Paper 490f:** A Computational Study on H<sub>2</sub> Absorption in a Porous Framework Structure or: The Curse of the Exponential Function — **Cheng-chau Chiu**, *Nguyen Minh Thong Le, Amol Deshmukh, Jer-Lai Kuo*

**2:30 Paper 490g:** Towards an Ultrasensitive Method for the Quantification of Metal Ions Using Surface-Enhanced Infrared Absorption Spectroscopy — **Xuan Yang**, *Marco Dunwell, Yushan Yan, Bingjun Xu*

#### **(491) Advanced Polymeric Membranes for Gas Separation**

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 303

Dhaval Bhandari, Co-Chair  
Alexander Lopez, Co-Chair  
Lingxiang Zhu, Co-Chair

**Sponsored by:** Membrane-Based Separations

**12:30 Paper 491a:** Sorption in PIM-1 from Cryogenic to Room Temperature: Experimental and Model Analysis — **Matteo Minelli**, *Brian R. Pimentel, Melinda L. Jue, Ryan Lively, Giulio C. Sarti*

**12:51 Paper 491b:** Highly Permeable and Selective Crosslinked Polybenzoxazole (PBO) Membranes for Gas Separation — **Gregory Kline**, *Ruilan Guo*



**1:12 Paper 491c:** Polybenzimidazole-Derived Carbon Molecular Sieves with Microcavities and Ultra-Microporous Channels Achieving Superior Membrane H<sub>2</sub>/CO<sub>2</sub> Separation Properties — *Maryam Omidvar, Haiqing Lin*

**1:33 Paper 491d:** Ultra-Selective Defect-Free Interfacially Polymerized Molecular Sieve Thin-Film Composite Membranes — *Zain Ali, Federico Pacheco, Eric Litwiller, Yingge Wang, Yu Han, Ingo Pinnau*

**1:54 Paper 491e:** Gas Sorption Properties of Novel Iptycene-Based Thermally Rearranged Co-Polymers: Effect of Temperature, Mixed Gas and Pre-Treatment — *Valerio Loianno, Shuangjiang Luo, Qinnan Zhang, Ruilan Guo, Michele Galizia*

**2:15 Paper 491f:** Synthesis and Multicomponent Permeation Evaluation of Functionalized PDMS Membranes for Enhanced NGL Recovery from Natural Gas — *John Yang, Daniel J. Harrigan, Milind Vaidya*

**2:36 Paper 491g:** A Scalable Method to Synthesize Zeolitic-Imidazolate Framework ZIF-8 Membranes on Polymer Hollow Fibers for Propylene/Propane Separation — *Mohamad Rezi Abdul Hamid, Hae-Kwon Jeong*

#### (492) Advances in Life Cycle Optimization for Process Development

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 320

Gonzalo Guillén-Gosálbez, Chair  
Debalina Sengupta, Co-Chair  
José M. Ponce, Co-Chair

**Sponsored by:** Process Development

**12:30 Paper 492a:** A Mathematical Programming Model for the Integration of Power Plants Involving Chemical Looping Combustion with Algal Systems Under Carbon Policies Analysis — *Aurora del Carmen Munguía-López, Vicente Rico-Ramírez, José María Ponce-Ortega*

**12:51 Break**

**1:12 Paper 492c:** A Framework for Multiscale Consequential Life Cycle Assessment — *Tapajyoti Ghosh, Bhavik R. Bakshi*

**1:33 Paper 492d:** Integrated Network Optimization and Uncertainty Analysis Streamlined LCA Method for the Petrochemical Industry — *Raul Calvo-Serrano, Gonzalo Guillén-Gosálbez,*

**(493) Advances in Processing and Handling of Energetic Materials**  
**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 414

Travis R. Sippel, Chair  
Lori J. Groven, Co-Chair

**Sponsored by:** Energetics

**12:30** Introductory Remarks

**12:35 Paper 493a:** High Surface Area Silicon Quantum Dots Derived from Porous Silicon for Energetic Materials — *Philip M. Guerieri, Sarah Adams, Nicholas Piekiet, Matthew Ervin, Wayne A. Churaman, Christopher Morris*

**12:55 Paper 493b:** A Materials Science-Based Approach for the Re-Development of COMP B — *Hongwei Qiu, Philip Samuels, Erik Wrobel, Aleksander Gandzelko, Victor Stepanov, Rajen B. Patel, Katherine H. Guarini*

**1:15 Paper 493c:** Replacement of Barium Chromate in the Traditional Tungsten Delay — *Lori J. Groven, Barbara A. Hadraza*

**1:35 Break**

**1:50 Paper 493d:** Combustion of Multi-Stage Ball Milled Ternary B/Al/PTFE Nano-Sale Composites — *Liyun Feng, Travis R. Sippel*

**2:10 Paper 493e:** Milling of Energetic Crystals with the Labram — *Lance Kotter, Lori J. Groven*

**2:30** Panel Discussion

#### (494) Atmospheric Chemistry and Physics II

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 319

Kristina Wagstrom, Chair  
Shunsuke Nakao, Co-Chair

**Sponsored by:** Air

**12:30 Paper 494a:** Study on Regional Air-Quality Impacted By Chemical Plant Shutdown Under the Lower Destruction and Removal Efficiency for Flare Combustion — *Sijie Ge, Sujing Wang, Qiang Xu, Thomas Ho*

**12:50 Paper 494b:** Physical and Chemical Aging of Carbonaceous Aerosol in the Eastern Mediterranean — *Antonios Tasoglou, Kalliopi Florou, Evangelos Louvaris, Aikaterini Liangou, Georges Saliba, Spyros N. Pandis*

**1:10 Paper 494c:** Global Source Apportionment of Atmospheric Particulate Matter — *Carmen Lamancusa, Kristina Wagstrom*

**1:30 Paper 494d:** The Impact of Vapor Supersaturation on the Morphology, Mixing State and Optical Properties of Atmospheric Soot — *Ogochukwu Enekwizu, Chao Chen, Gennady Gor, Christopher D. Dobrzanski, Alexei Khalizov*

**1:50 Paper 494e:** The Competition between Surface and Capillary Condensation of Vapors on Soot Aggregates — *Ella Ivanova, Alexei Khalizov, Gennady Gor*

**2:10 Paper 494f:** From Nascent to Mature Soot Light Absorption during Agglomeration and Surface Growth — *Georgios A. Kelesidis, Sotiris E. Pratsinis*

#### (495) Biomass Thermal Deconstruction via Fast Pyrolysis Biorefineries

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 316

Robert C. Brown, Chair  
Mark Mba Wright, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**12:30 Paper 495a:** Condensed Phase Reactions of Polysaccharides during Fast Pyrolysis — *Jake K. Lindstrom, Chad Peterson, Patrick A. Johnston, Peter N. Ciesielski, Preston A. Gable, Robert C. Brown*

**12:55 Paper 495b:** Origins of Enhanced Levoglucosan Yields during the Co-Pyrolysis of Cellulose and High-Density Polyethylene — *Melisa Nallar, Hsi-Wu Wong*

**1:20 Paper 495c:** Understanding Fast Pyrolysis of Microalgae Model Components Via Py-FTIR and Py-GCMS — *Ribhu Gautam, R. Vinu*

**1:45 Paper 495d:** Renewable Materials from Catalytic Fast Pyrolysis — *Mark R. Nimlos, Nolan Wilson, Christopher Kinchin, Calvin Mukarakate*

**2:10 Paper 495e:** The Effects of Pretreatments in Improving the Quality of Bio-Oil Products from Non-Catalytic and Catalytic Pyrolysis of Lignocellulosic Biomass — *Roosbeh Seifollahy-Astaraee, Charles Coe, Justinus A. Satrio*

**(496) Biomaterial Scaffolds for Tissue Engineering I: Musculoskeletal Applications**  
**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 328

Ryan Koppes, Co-Chair  
Jungwoo Lee, Co-Chair  
Tadas Kasputis, Co-Chair

**Sponsored by:** Biomaterials

**12:30 Paper 496a:** Demineralized Bone Slices for in Vitro Endosteal Niche Modeling — *Yongkuk Park, Ryan Carpenter, Jungwoo Lee*

**12:48 Paper 496b:** Defining the Mechanisms of Immune Resolution after Biomaterial Implant into Adipose Tissue — *Kendall Murphy, Michael Gower*

**1:06 Paper 496c:** A Poly-L-Lactide Scaffold with Continuous Gradient Pore Size That Differentially Induce Local Chondrogenesis and Osteogenesis for Osteochondral Repair — *Riccardo Gottardi, Gioacchino Conoscenti, Peter Alexander, Vincenzo La Carrubba, Valerio Brucato, Rocky Tuan*

**1:24 Paper 496d:** BMP-2 Conjugated Micro-Fiber/Hydrogel Composites for Bone Integration to Engineered Ligament Tissue — *Dina Gadalla, Patrick Thayer, Aaron S. Goldstein*

**1:42 Paper 496e:** Human Skeletal Muscle Growth and Maturation in 3-Dimensional Silk-Extracellular Matrix Scaffolds — *Schuyler S. Link, Raul G. Cruz Quintero, Juliana A. Passipieri, George J. Christ, Lauren D. Black III, David L. Kaplan, Whitney L. Stoppel*

**2:00 Paper 496f:** 3D Graphene Foam Based Scaffolds to Control Transdifferentiation of MSCs into Schwann Cell-like Phenotypes Via Electrical Stimuli for Peripheral Nerve Regeneration — *Metin Uz, Ju Jung Hyung, Surya K. Mallapragada, Piran Kidambi, Donald S. Sakaguchi*

**2:18 Paper 496g:** Nanofibrous Scaffolds Produced By Electrospinning, Rotary-Jet Spinning and Airbrush for Orthopedic Tissue Regeneration — *Paria Ghannadian, James W. Moxley Jr., Mirian De Paula, Thomas J. Webster*

**2:36 Paper 496h:** Tissue Origami for Biomineralization — *Gulden Camci-Unal*



**(497) Biomolecules at Interfaces II  
Wednesday, Oct 31, 12:30 PM**

Omni William Penn Hotel, Conference Center B

Susan Daniel, Chair  
Bernardo Yanez Soto, Co-Chair  
Amir M. Farnoud, Co-Chair**Sponsored by:** Interfacial Phenomena**12:30 Paper 497a:** Detailed Molecular Models of Interfacial Proteins from Sum Frequency Generation Spectroscopy — **Vance Jaeger, Helmut Lutz, Tobias Weidner, Bert de Groot****12:45 Paper 497b:** Elucidating Protein Corona Formation on Nanoparticles in Complex Biological Fluids — **Rebecca Pinals, Markita Landry****1:00 Paper 497c:** X-Ray Reflectivity and Pendant Drop Tensiometry Measurements of the Competitive Adsorption of Mabs and Excipients at the Air-Water Interface — **Ankit Kanthe, Mary Krause, Songyan Zheng, Binhua Lin, Wei Bu, Joseph Strzalka, Charles Maldarelli, Raymond Tu****1:15 Paper 497d:** Why Do Surface and Solution Hybridization Differ? — **Rastislav Levicky, Hao-Chun Chiang****1:30 Paper 497e:** Design of a Cholesterol-Binding Peptide to Inhibit Bacterial Toxin Activity — **Evan Koufos, Angela C. Brown****1:45 Paper 497f:** Explaining Catechol-Cation Binding Synergy with Bond Energies and Lifetimes — **George Degen, Roberto C Andresen Eguiluz, Robert Lewis, Alison Butler, Jacob Israelachvili****2:00 Paper 497g:** Mussel-Inspired Peptoids: The Backbone's Role in Adhesive Properties — **Thomas R. Cristiani, William Wonderly, George Degen, Keila Cunha E Silva, Joan-Emma Shea, J. Herbert Waite, Jacob Israelachvili****2:15 Paper 497h:** Characterization of the Aqueous Dispersion of Boron Nitride Nanotubes Stabilized By DNA — **Venkateswara Rao Kode, Camerin McDonald, John Weicherding, Tony Dobrila, Petru S. Fodor, Christopher L. Wirth, Geyou Ao****(498) Bionanotechnology for Gene and Drug Delivery I  
Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 309

Elizabeth Nance, Chair  
Joo-Youp Lee, Co-Chair**Sponsored by:** Bionanotechnology**12:30 Paper 498a:** Invited Speaker: Exciton Engineering for Brain Nanosensor Delivery, and Imaging of Modulatory Neurotransmitters — **Abraham Beyene, Jackson Travis Del Bonis-O'Donnell, Kristen Delevich, Markita Landry****1:00 Paper 498b:** Biodistribution and Drug Release Kinetics of Gold Nanoconjugates for Respiratory Recovery after Spinal Cord Injury — **Fangchao Liu, Janelle Buttry, Zeljka Minic, Harry G. Goshgarian, Guangzhao Mao****1:18 Paper 498c:** Liposomes Functionalized with Cell-Penetrating Peptides As a Novel Treatment for Bacterial Meningitis — **Caterina Bartomeu Garcia, Di Shi, Thomas Webster****1:36 Paper 498d:** Uncorking and Oxidative Decomposition Dynamics of Gold Nanoparticle Corked Carbon Nanotube Cups for Drug Delivery Studied *Via in Situ* Transmission Electron Microscopy — **Stephen House, Christopher M. Andolina, Seth Burkert, Alexander Star, Judith C. Yang****1:54 Paper 498e:** Length-Dependent Uptake, Inflammation, and Intracellular Processing of Single-Walled Carbon Nanotubes in Macrophages — **Sumin Jin, Piyumi Wijesekara-Kankanange, Patrick D. Boyer, Kris Noel Dahl, Mohammad F. Islam****2:12 Paper 498f:** Nanoparticle Optimization for Improved Vaginal Drug Delivery during Pregnancy — **Hannah Zierden, Victoria Laney, Sabrina Bensouda, Kevin DeLong, Fareeha Zulfiqar, Thuy Hoang, Yujie Zou, Jamie Maziarz, Mala Mahendroo, Gunter Wagner, Justin Hanes, Laura Ensign****2:30 Paper 498g:** Responsive Foams for Nanoparticle Delivery — **Chang Tian, Christina Tang, Antoinette Nelson, Jennifer Holloway, Patrick J. Sinko, Robert K. Prud'homme****(499) Bioseparations and Downstream Processing  
Wednesday, Oct 31, 12:30 PM**

Westin Convention Center, Somerset

Zifan Gong, Chair  
Jiali Du, Co-Chair**Sponsored by:** Bioengineering**12:30 Paper 499a:** Purification of Exosomes Using Tangential Flow Filtration — **Eric Plencner, Jeffrey J. Chalmers****12:48 Paper 499b:** Model-Based Optimization and Design of Continuous Chromatography for Protein Capture — **Ce Shi, Zong-Ye Gao, Shan-Jing Yao, Dong-Qiang Lin****1:06 Paper 499c:** Sterile Filtration of Oncolytic Viruses Using Novel Nanoporous Silicon Nitride Membranes — **Evan Wright, Shabnam Shoaebargh, Josh Miller, Jeff Rowan, Adam Smith, Joris Van der Heijden, James Roussie, James McGrath, David Latulippe****1:24 Paper 499e:** Docking Simulations to Predict Binding Performance of Affinity Ligands for Purification of Butyrylcholinesterase — **Rudra Palash Mukherjee, Benjamin G. Bobay, Geok-Yong Yow, Samuel Sarakbi, Patrick V. Gurgel, Ruben G. Carbonell****1:42 Paper 499f:** Computational Design of Peptide Ligands for the Bioseparation of "Fab" Antibody Fragments — **Xingqing Xiao, Hannah Reese, Stefano Menegatti, Carol Hall****2:00 Paper 499g:** Downstream Processing in Biomanufacturing: Multimodal Chromatography, Affinity Precipitation and Integrated Bioprocessing — **Steven Cramer****(500) Catalysis for C1 Chemistry II: Methane Reforming and Oxidation  
Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 403

Dolly Chitta, Chair  
Ambarish R. Kulkarni, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**12:30 Paper 500a:** Non-Oxidative Conversion of Methane into Light Hydrocarbons Using Single-Atom Platinum Catalysts — **Chao Wang****12:48 Paper 500b:** Highly Selective Nonoxidative Coupling of Methane (NOCM) over Pt-Bi Bimetallic Catalysts — **Yang Xiao, Arvind Varma****1:06 Paper 500c:** Oxidative Coupling of Methane: The Role of the Tungstate Promoter in Mn-Na<sub>2</sub>WO<sub>4</sub> — **Gizem Ozbuyukkaya, Goetz Vesper****1:24 Paper 500d:** Microkinetic Modeling of Direct, Non-Oxidative Conversion of Methane to Value-Added Chemicals over Iron/Silica Catalyst — **Hilal Ezgi Toraman, Konstantinos Alexopoulos, Dionisios G. Vlachos****1:42 Paper 500e:** Co-Aromatization of Methane with Propane over Zn/HZSM-5: The Methane Reaction Pathway and the Effect of Zn Distribution — **Peng He, Jack Jarvis, Shijun Meng, Hua Song****2:00 Paper 500f:** Catalytic Aromatization of Methane: Strategies for Improving Active Chemistry and Stability of the Catalysts — **Sheima J. Khatib, Mustafizur Rahman, Apoorva Sridhar****2:18 Paper 500g:** Performance and Phase Stability Studies of Gadolinium-Doped Barium Cerate in Oxidative Coupling of Methane and the Impact of Zr Doping — **Valentina Omoze Igenegbaji, Randall J. Meyer, Suljo Linic****2:36 Paper 500h:** Effects of Controlled Crystalline Surface of Hydroxyapatite on Methane Oxidation Reactions — **Su Cheun Oh, Dongxia Liu****(501) Catalysis with Microporous and Mesoporous Materials II: Site Specific and Mechanistic Characterization  
Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 404

Xueyi Zhang, Chair  
Praveen Bollini, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**12:30 Paper 501a:** Pt Encapsulated within Small-Pore Zeolites for Selective H<sub>2</sub> Scavenging during Dehydrogenation of Light Alkanes — **Haefa Mansour, Enrique Iglesia****12:50 Paper 501b:** Spatial Characterization of Solid Acid Catalysts By Reactive Gas Chromatography — **Paul J. Dauenhauer, Katherine P. Vinter, Omar A. Abdelrahman****1:10 Paper 501c:** Speciation of Liquid Ion-Exchanged Cu into SSZ-13, ZSM-5, and Beta Zeolites — **Arthur J. Shih, Juan M. Gonzalez, Ishant Khurana, Lucia Pérez Ramirez, Andres Peña L., Aleksey Yezerets, Rajamani Gounder, Aida Luz Villa, Fabio H. Ribeiro****1:30 Paper 501d:** Quantitative Attenuated Total Reflection Infrared Spectroscopy for Understanding Solvent Effects in Liquid Phase Reactions on Zeolites — **Nicholas Gould, Bingjun Xu**

**1:50 Paper 501e:** First-Principles Development of AI Proximity Titration Strategy for SSZ-13 Zeolite through Comparison of Divalent Metal Cation Exchange Energy Landscapes — **Sichi Li**, Casey Jones, John R. Di Iorio, Anthony DeBellis, Imke Britta Mueller, Rajamani Gounder, William F. Schneider

**2:10 Paper 501f:** Investigating the Effect of Si/Al Ratio on the Catalytic Activity of Two-Dimensional MFI Nanosheets in Friedel-Crafts Alkylations Employing Bulky Reactants — **Akshay Korde**, Byunghyun Min, Sankar Nair, Christopher W. Jones

**2:30 Paper 501g:** Improving Methanol-to-Olefins Turnover Capacity of CHA Materials By Controlling Methanol Transfer Dehydrogenation Rates — **Praveen Bollini**, Aditya Bhan

## (502) Combinatorial Techniques in Protein Engineering

**Wednesday, Oct 31, 12:30 PM**  
Westin Convention Center,  
Westmoreland East

Arnab Mukherjee, Chair  
Jerome M. Fox, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 502a:** Biomolecular Engineering of Acoustomagnetic Protein Nanostructures for Non-Invasive Imaging of Cellular Function — **George J. Lu**, Arash Farhadi, Jerzy O. Szablowski, Audrey Lee-Gosselin, Samuel R. Barnes, Anupama Lakshmanan, Raymond W. Bourdeau, Mikhail G. Shapir

**12:48 Paper 502b:** Synthetic Electron Transfer Pathways As High-Throughput Selections for the Design of Protein Electron Carriers — **Jonathan J.**

**Silberg**

**1:06 Paper 502c:** Automating the Engineering of Improved Enzymes for Biomanufacturing — **Emily Wrenbeck**, Matt Bedewitz, Raisa Noshin, **Tim Whitehead**

**1:24 Paper 502d:** Constrained Combinatorial Libraries of Gp2 Proteins Enhance Discovery of Synthetic PD-L1 Ligands — **Benjamin J. Hackel**, Max A. Kruziki, Vidur Sarma

**1:42 Paper 502e:** Design of Glycosylation Sites By Rapid Synthesis and Analysis of Glycosyltransferases — **Weston Kightlinger**, Liang Lin, Madisen Rosztoczy, Wenhao Li, Matthew P. DeLisa, Milan Mrksich, Michael C. Jewett

**2:00 Paper 502f:** Elucidating the Evolvability of Ancestral Proteins Using a Continuous Stirred Tank Bioreactor — **Daniel R. Woldring**, Christopher Wilson, Chiquita McCoy-Crisp, Brandon Black, Dorothee Kern

**2:18 Paper 502g:** Synthetic Genetic Systems for Rapid Mutation and Evolution *In Vivo* — **Chang Liu**

## (503) Complex Fluids: Macromolecules

**Wednesday, Oct 31, 12:30 PM**  
Omni William Penn Hotel, Frick

Nicolas J. Alvarez, Chair  
Simon Rogers, Co-Chair

**Sponsored by:** Fluid Mechanics

**12:30 Paper 503a:** Internal Dynamic Modes and Rheology of Cellulose Nanofibrils with Salt — **Sara M. Hashmi**, Gilad Kaufman, Nawal Quennouz, Chinedum O. Osuji

**12:45 Paper 503b:** Visualization of Polymer Dynamics of Highly Entangled Shear-Banding Polymer Solutions Under Large Amplitude Oscillatory Shear (LAOS) — **Seunghwan Shin**, Kevin D. Dorfman, Xiang Cheng

**1:00 Paper 503c:** Uniaxial Extension of Associative Proteins Reveals Chain Alignment Mechanism in Highly Extensible and Tough Protein Hydrogels — **Chelsea Edwards**, **Danielle J. Mai**, Shengchang Tang, Bradley D. Olsen

**1:15 Paper 503d:** Branching and Alignment in Reverse Worm-like Micelles Studied with Simultaneous Dielectric Spectroscopy and Rheosans — **John K. Riley**, Jeffrey J. Richards, Norman J. Wagner, Paul Butler

**1:30 Break**

**1:45 Paper 503f:** Elasto-Inertial Turbulence: Reentrant Transition and Connection to Linear Mechanisms — **Ashwin Shekar**, Ryan McMullen, Sung-Ning Wang, Beverley McKeon, Michael D. Graham

**2:00 Paper 503g:** Single Molecule Studies of Comb Polymer Dynamics in Semi-Dilute Solutions — **Shivani F. Patel**, Charles M. Schroeder

**2:15 Paper 503h:** Transient Evolution of Shear Bands in a Model Wormlike Micellar Solutions — **Alireza Dalili**, **Hadi Mohammadigoushki**

**2:30 Paper 503i:** A Direct Correlation between Recoverable Strain and Microstructural Evolution of Wormlike Micelles out of Equilibrium — **Ching-Wei Lee**, **Simon Rogers**

**2:45 Paper 503j:** Impact of Polymer Binder on Battery Slurry Rheology and Electrode Performance — **Samantha L. Morelly**, Maureen H. Tang, Nicolas J. Alvarez

## (504) Computational Catalysis V: Oxides, Zeolites, Porous Catalysts, and Supported Catalysts

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center,  
402

Chris Paolucci, Chair  
Hui Li, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 504a:** Examination of Brønsted and Lewis Acid-Catalyzed Alkane Reactions in MFI Zeolites Using a Hybrid QM/MM Scheme — **Erum Mansoor**, Martin Head-Gordon, Alexis T. Bell

**12:48 Paper 504b:** First Principles Modeling of Extended Solvent Structures in Defected Microporous Materials and Their Influence on the Kinetics of Lewis Acid Site Speciation — **Brandon C. Bukowski**, Jason S. Bates, Rajamani Gounder, Jeffrey Greeley

**1:06 Paper 504c:** Computational Screening of Metal-Organic Frameworks for Direct Methane to Methanol Conversion — **Hieu A. Doan**, Benjamin Bucior, Randall Q. Snurr

**1:24 Paper 504d:** Computational Prediction of the Structure and Catalytic Properties of Copper Zirconium Oxide — **James Dean**, **Giannis Mpourmpakis**

**1:42 Paper 504e:** Elucidating the Role of Oxygen Coverage in CO<sub>2</sub> Reduction on Mo<sub>2</sub>C — **Mudit Dixit**, Xi Peng, Marc D. Porosoff, **Giannis Mpourmpakis**, Heather D. Willauer

**2:00 Paper 504f:** Balancing Reactivity and Stability in Metal Nanoparticle and Alumina Support Systems Via Redox Reactions: A Multiscale Computational and Experimental Approach — **Matthew Curnan**, Henry Ayoola, Matthew McCann, Wissam A. Saidi, Judith C. Yang

**2:18 Paper 504g:** Understanding the Role of Promoters for Propane Dehydrogenation Catalysts — **Zhi-Jian Zhao**, Jinlong Gong

**2:36 Paper 504h:** A Theoretical Examination of Nitrogen Photofixation on Rutile TiO<sub>2</sub>(110) — **Benjamin Comer**, Andrew Medford

## (505) Continuous Processing Technologies Applied in Drug Product Development I

**Wednesday, Oct 31, 12:30 PM**  
Westin Convention Center, Washington

Joe Hannon, Chair  
Elcin Icten, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**12:30 Paper 505a:** Development and Qualification of a Custom Continuous Blending System for Clinical Manufacturing — **Daniel Borginis**

**12:51 Paper 505b:** Feeder Discharge Prediction Using Discrete Element Method (DEM) Simulations — **Martina Trogrlic**, Peter Toson, Eva Siegmann, Dalibor Jajcevic, Johannes G. Khinast, Pankaj Doshi, Daniel O. Blackwood, Mary T. am Ende

**1:12 Paper 505c:** Towards Continuous Manufacturing (CM) of Drug Loaded Strip Films: Continuous Mixing of Dry Micronized Drug Particles with Film Precursor Via Twin Screw Extruder (TSE) — **Guluzar Gorkem Buyukgoz**, Jeremiah Castro, Kasinathan Velmurugan, Rajesh Davé

**1:33 Paper 505d:** Material Properties Characterization and Ingredient Agglomerate Behavior in Continuous Direct Compaction Process — **Zhanjie Liu**, Gerardo Callegari, Qiushi Zhou, Fernando J. Muzzio

**1:54 Paper 505e:** Comparing a Semi-Continuous Tablet Coating Process at Different Scales Using CFD-DEM — **Peter Böhling**, Wen-Kai Hsiao, Frederik Detobel, James Holman, Laura Wareham, Johannes G. Khinast, **Matthew Metzger**

**2:15 Paper 505f:** Continuous Fluidized Bed Drying of Pharmaceutical Granulations: Prediction of the Moisture Content — **Hao Chen**, Subham Rustagi, Emily Diep, Tim A. G. Langrish, Benjamin J. Glasser

**2:36 Paper 505g:** SEMI-Continuous Manufacturing Process for Generic Drug Products — **Ajay Babu Pazhayattil**, Naheed Sayeed-Desta

**(506) CO<sub>2</sub> Capture By Adsorption**  
**Wednesday, Oct 31, 12:30 PM**  
 David L. Lawrence Convention Center, 334

Youssef Belmabkhout, Chair  
 Enzo Mangano, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**12:30 Paper 506a:** CO<sub>2</sub> Extraction from Simulated Air Via Temperature Swing Adsorption Using Polymer/Silica Fiber Sorbents — **Achintya Sujan, Simon H. Pang, Guanghui Zhu, Christopher W. Jones, Ryan Lively**

**12:52 Paper 506b:** Direct Air Capture of CO<sub>2</sub> Using Zeolites — **Sean Wilson, F. Handan Tezel**

**1:14 Paper 506c:** Silica Supported Poly(Propylene Guanidine) for CO<sub>2</sub> Capture in Simulated Flue Gas and Ambient Air — **Sang Jae Park, Caroline Hoyt, Christopher Jones**

**1:36 Paper 506d:** Development of Advanced Solid Sorbent for CO<sub>2</sub> Capture from Flue Gas — **Xiaoxing Wang, Chunshan Song**

**1:58 Paper 506e:** Improved CO<sub>2</sub> Selectivity-Uptake Trade-Off Driven by Synergetic Thermodynamics, Kinetics, and Packing Effects — **Youssef Belmabkhout**

**2:20 Paper 506f:** Impregnation of Hydrotalcite with NaNO<sub>3</sub> for Enhancement of CO<sub>2</sub> Sorption Uptake — **Suji Kim, Ki Bong Lee**

**2:42 Paper 506g:** Preparation and Its Excellent CO<sub>2</sub>/CH<sub>4</sub>/N<sub>2</sub> Adsorption Selectivity of Novel Carbon Composites CPDA@A-ACs — **Wanwen Liang, Huiyu Xiao, Zhong Li**

**(507) Developing Process Control Strategies for Drug Product Manufacture**

**Wednesday, Oct 31, 12:30 PM**  
 Westin Convention Center, Fayette

Dominique Hebrault, Chair  
 Kevin Stone, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**12:30 Paper 507a:** A Hybrid Process Control System for Fluidized Bed Drug Layering Process — **Hanzhou Feng, James K. Drennen III, Carl A. Anderson**

**12:51 Paper 507b:** Application of Mechanistic Models for the Digital Design and Online Control of Pharmaceutical Processes — **Niall Mitchell, John Mack, Furqan Tahir**

**1:12 Paper 507c:** Impact of Physico-Mechanical Properties of Co-Processed Excipients on the Tableting Performance By DM3 Approach — **Nikita Patil, Abhay Jain, Scott Staton, Rahul Haware**

**1:33 Paper 507d:** Pharmacy on Demand: On-Demand Drug Product Manufacturing in a Miniaturized and Portable System — **Mohammad Azad, Juan G. Osorio, David Brancazio, Gregory Hammersmith, David Klee, Kersten Rapp, Allan Myerson**

**1:54 Paper 507e:** Applying Dynamic Similarity Principles to a Narrow Therapeutic Index Drug Powder Blending Process Scale-up: Laboratory Case Studies and Relevant Regulatory Experience — **Huiquan Wu, Koushik Sowrirajan, Masihuddin Jaiqirdar**

**2:15 Paper 507f:** Implementation of Advanced Process Control System into Continuous Pharmaceutical Manufacturing Pilot-Plant — **Ravendra Singh**

**2:36 Paper 507g:** The Role of Software Tools in Quality By Design: A Case Study on Monoclonal Antibody Production — **Maria M. Papathanasiou, Nilay Shah, Efstratios N. Pistikopoulos**

**(508) Development of Intermolecular Potential Models**

**Wednesday, Oct 31, 12:30 PM**  
 David L. Lawrence Convention Center, 307

Neeraj Rai, Chair  
 Shuangliang Zhao, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**12:30 Paper 508a:** Development of Force Fields to Model Upcoming 2D Materials in Mechanical and Interfacial Applications — **Ananth Govind Rajan, Vishnu Sresht, Agilio A. H. Pádua, Michael Strano, Daniel Blankschtein**

**12:48 Paper 508b:** Accurate Simulation of Oxides and Hydroxides up to the Large Nanometer Scale — **Krishan Kanhaiya, Michael Nathanson, Hendrik Heinz**

**1:06 Paper 508c:** The Quantum Mechanics Based Polarizable Force Field for Simulations of Complex Materials: Application to Water System — **Saber Naserifar, William A. Goddard III**

**1:24 Paper 508d:** Computing Virial Coefficients to Assess the Accuracy of Intermolecular Potentials — **Navneeth Gokul, Andrew J. Schultz, David A. Kofke**

**1:42 Paper 508e:** Molecular Origin of Robeson Limit in across-Membrane Transport — **Jiabo Tao, Shuangliang Zhao, Xiaohua Lu, Honglai Liu**

**2:00 Paper 508f:** Bayesian Inference Demonstrates Inadequacies of Mie *N*-6 Repulsive Barrier at High Pressures — **Richard A. Messerly, Andrei Kazakov**

**2:18 Paper 508g:** Systematic Refinement of Gaff Force Field for Nineteen Organic Battery Electrolytes — **Yushan Zhang, Yong Zhang, Alexander W. Dowling, Mark J. McCready, Edward J. Maginn**

**2:36 Paper 508h:** Calorimetric and Spectroscopic Studies on the Interaction between Angiotensin Converting Enzyme (ACE) Inhibiting Peptide GMKCAF and ACE — **Xiongdao Lan, Lixia Sun, Zefen Wang, Liqin Zhou, Jianhua Sun, Zhangfa Tong, Shuangfei Wang, Dankui Liao**

**(509) Drug Delivery II: Small Molecules**

**Wednesday, Oct 31, 12:30 PM**  
 Westin Convention Center, Cambria

Greg Thurber, Chair  
 Srivatsan Kidambi, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**12:30 Paper 509a:** Ultrahigh and Multiple Anti-Tuberculosis Drugs Loaded BioMOFs Clear Mycobacterium Tuberculosis Infection in Macrophages — **Abhinav P. Acharya, Ashlee Greene, Kutay Berk Sezginel, Christopher E. Wilmer, Steven Little**

**12:48 Paper 509b:** Biohybrid Microswimmers with Biocompatible Polymeric Multilayers As Drug Delivery System — **Byung-Wook Park, Guraarashjot S Multani, Katelyn M Bevilacqua, Jonathan J Caguiat, Douglas M Price**

**1:06 Paper 509c:** Antibiotic-Dispersion Aerosols for Enhanced Eradication of *Pseudomonas Aeruginosa* biofilms — **Jennifer Fiegel, Sachin Gharse**

**1:24 Paper 509d:** Polyampholyte Microspheres for Extended Drug Delivery — **Emily Mariner, Matthew T Bernards**

**1:42 Paper 509e:** Macromolecular Engineering in Silicone Hydrogel Contact Lenses for the Controlled Release of Multiple Small Molecules — **Stephen A. DiPasquale, Biaggio Uricoli, Matthew C. DiCerno, Mark E. Byrne**

**2:00 Paper 509f:** Targeted Delivery of a Theophylline Coupled Nanoconjugate Induces Recovery of the Diaphragm Following Cervical Spinal Cord Injury in Rats — **Fangchao Liu, Janelle Buttry, Zeljka Minic, Harry G. Goshgarian, Guangzhao Mao**

**2:18 Paper 509g:** Electrospun Patch for Transdermal Delivery of Contraceptive Hormone — **Mohammad Mofidfar, Mark R. Prausnitz**

**2:36 Paper 509h:** The Effect of Chitosan Surface Modification on PLGA Vascular Adhesion and Protein Adsorption for Improved Drug Delivery Systems — **Genesis Lopez-Cazares, Omolola Eniola-Adefeso**

**(510) Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions I**

**Wednesday, Oct 31, 12:30 PM**  
 David L. Lawrence Convention Center, 306

Gang Wu, Chair  
 Hong Yang, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

**12:30 Paper 510a:** U.S. Department of Energy Early-Stage Alkaline Membrane Fuel Cell R&D (Invited) — **Simon T. Thompson, Donna Ho, Dimitrios Papageorgopoulos**

**12:50 Paper 510b:** Bifunctional Catalyst Enabled Reversible Fuel Cells for Energy Storage (Invited) — **Hui Xu**

**1:10 Paper 510c:** Ultra-Low PGM and PGM-Free High-Performance Electrodes for Aemfcs — **Xiong Peng, Travis Omasta, Emanuele Magliocca, William E. Mustain**

**1:30 Paper 510d:** Addressing Transport Losses in Low-Pt and Pt-Free PEM Fuel Cell Cathodes (Invited) — **Shawn Litster**

**1:50 Paper 510e:** Electrocatalyst Development for Active and Durable Oxygen Evolution Reaction (Invited) — **Zhenmeng Peng**

**2:10 Paper 510f:** Mechanistic Insights into the Active Sites and Their Local Environments for Electrocatalytic Reduction Systems (Invited) — **Matthew Neurock**



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.



**2:30 Paper 510g:** Degradation Mechanisms of PEM Water Electrolysis MEA after Long-Term Operation (Invited) — *Haoran Yu, Leonard Bonville, Radenka Maric*

**2:50 Paper 510h:** Electrocatalytic Conversion of Energy Molecules with 2D Materials (Invited) — *Dehui Deng*

### (511) Electrochemical Reactors, Fuel Cells, and Electrolyzers II

**Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 323

Al Sacco Jr., Chair  
Jamie Holladay, Co-Chair  
Michael Sees, Co-Chair

**Sponsored by:** Alternate Fuels and New Technology

**12:30 Paper 511a:** Design of the Self-Humidifying Membrane Electrode Assembly Employing Direct Membrane Deposition Technique for Fuel Cell —

**12:55 Paper 511b:** Nature-Inspired Flow-Fields and Water Management for PEM Fuel Cells — *Jason Cho, Tobias Neville, Panagiotis Trogadas, Billy Wu, Dan Brett, Marc-Olivier Coppens*

**1:20 Paper 511c:** Electrospun Particle/ Polymer Fiber Mats As Hydrogen/ Air Fuel Cell Electrodes — *Krysta Waldrop, John Slack, Ryszard Wycisk, Peter N. Pintaro*

**1:45 Paper 511d:** Electrocatalytic Hydrogenation of Biogenic Compounds: Reaction Networks and Mechanisms — *Oliver Gutiérrez, Udishnu Sanyal, Laura Meyer, Jamie Holladay, Johannes A. Lercher*

**2:10 Paper 511e:** Chemical Transformations Using Electrocatalysis: From Small Molecules to Fast Pyrolysis Oils — *Jamie Holladay, Juan A. Lopez-Ruiz, Jonathan Egbert, Asanga B. Padmaperuma*

**2:35 Paper 511f:** Selective Removal of Ethane and Natural Gas Liquids at the Well Pad Via Electrogenative Processing — *Maasoom Jafari, Samgopiraj Velraj, Jason Tremblay*

### (512) Emerging Junior Investigator Open Innovation Forum (Invited Talks)

**Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 331

Hyunmin Yi, Chair  
Jin Ryou Kim, Co-Chair  
Su Ha, Co-Chair  
Tae-Sik Oh, Co-Chair

**Sponsored by:** International Committee

**12:30 Paper 512a:** Photothermal Phase-Transition Nanodroplets and Their Drug Delivery Applications — *Yoonjee Park*

**12:55 Paper 512b:** Relaxation Processes and Dynamics of Ionic Liquids in Nanoconfined Geometries — *Younjin Min*

**1:20 Paper 512c:** Study of Catalytic NO+CO and Dry Reforming Reaction over CoO<sub>x</sub>/CeO<sub>2</sub>: Molecular and Electronic Structure-Activity Relationships — *Taejin Kim*

**1:45 Paper 512d:** In Vitro Recapitulation of Collective Dynamic Mucus Barrier Complexity — *Jungwoo Lee*

### (513) Emerging Tools and Enabling Technologies in Synthetic Biology: Sensors and Actuators

**Wednesday, Oct 31, 12:30 PM**

Westin Convention Center, Westmoreland West-Central

Nathan Crook, Co-Chair  
Kristin Adolfsen, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 513a:** Synthetic Organelles Engineered from Phase-Separating Proteins — *Benjamin S. Schuster, Ellen H. Reed, Holly Ramage, Matthew C. Good, Daniel A. Hammer*

**12:48 Paper 513b:** Engineering a Blue Light Inducible Spycatcher System (BLISS) As a Tool for the *in Vitro* Photo-Patterning of Proteins and Optically Controlled Intracellular Protein Activity — *Emily Hartzell, Justin Terr, Wilfred Chen*

**1:06 Paper 513c:** Sequence Specific Constraint-Based Modeling of *E. coli* Cell-Free Protein Synthesis — *Michael Vilkhovoy, Jeffery D. Varner*

**1:24 Paper 513d:** Cell-Free Systems for Equipment-Free Quantitation of Micronutrients in Human Serum — *Monica Mc Nerney, Mark P. Styczynski*

**1:42 Paper 513e:** Profiling Protease Substrate Specificity with Yess-NGS — *Carl A. Denard, Rasha Yaghi, Joseph Taft, Brent L. Iverson*

**2:00 Paper 513f:** Continuous Evolution of Engineered Synthetic Auxotrophs for Industrial Application — *Aditya M. Kunjapur, Michael G. Napolitano, Max Schubert, Evan Appleton, Karen Noguera, Daniel J. Mandell, George M Church*

**2:18 Paper 513g:** Dissecting the Genotype-to Phenotype Map in Eukaryotes: Molecular Determinants of Dominance, Heterosis, Pleiotropy, and Epistasis in Complex Traits — *Christopher M. Jakobson, Richard She, Daniel F. Jarosz*

**2:36 Paper 513h:** Tuning Extracellular Electron Transfer to Control Polymer Synthesis — *Christopher M. Dundas, Gang Fan, Austin J. Graham, Benjamin K. Keitz*

### (514) Fuel Processing for Hydrogen Production

**Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 321

Dushyant Shekhawat, Chair  
Daniel J. Haynes, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**12:30 Paper 514a:** Water-Gas Shift Reactor for Fuel Cell Systems: Stable Operation for 5000 Hours — *Joachim Pasel, Remzi Can Samsun, Andreas Tschauder, Ralf Peters, Detlef Stolten*

**12:49 Paper 514b:** Enhancements on Diesel Autothermal Reformer for Low-Temperature Solid Oxide Fuel Cell Integration — *Minseok Bae, Hyungjun Cheon, Jiwoo Oh, Joongmyeon Bae, Sai P. Katikaneni*

**1:08 Paper 514c:** Rapid Production of High-Purity Hydrogen Fuel from Liquid Hydrocarbon Fossil Fuels — *Xiangyu Jie, Peter P. Edwards, Tiancun Xiao*

**1:27 Paper 514d:** Hydrogen Production from Liquid Hydrocarbons with Process Intensification – a Case Study — *Jaemyung Lee, Jae Young Yoo, Joongmyeon Bae, Aadesh X. Harale, Sai P. Katikaneni*

**1:46 Paper 514e:** The Effect of Catalytic Metal on the Activity of Lanthanum Zirconate Pyrochlore Under Low S/C Methane Reforming Conditions — *Daniel J. Haynes, Dushyant Shekhawat, David Berry, James J. Spivey*

**2:05 Paper 514f:** Hydrogen Production through Diesel Steam Reforming: Process Intensification Using Structured Thermo-Neutral Reforming Catalyst — *Shakeel Ahmed, Sai P. Katikaneni, Aadesh X. Harale*

**2:24 Paper 514g:** High Temperature Catalyst Development and Testing for Low Cost and Efficient Solar Driven Sulfur-Based Hydrogen Production — *Birendra Adhikari, Daniel M. Ginosar, Fahim Rahman, Weijian Diao, John Meynard M. Tengco, John Monnier, Claudio Corgnale*

**2:43 Paper 514h:** Technoeconomic Study of Advanced H<sub>2</sub> Production Technologies: Membrane-Supported H<sub>2</sub>O Splitting, Thermochemical Redox H<sub>2</sub>O Splitting and Fuel-Assisted H<sub>2</sub>O Electrolysis — *Xiao-Yu Wu, Ahmed F. Ghoniem*

### (515) Graphene 2-D Materials: Synthesis, Functions and Applications I

**Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 310

Lei Li, Chair  
Sanjay Behura, Co-Chair

**Sponsored by:** Carbon Nanomaterials

**12:30 Paper 515a:** Effect of Hydrocarbon Contamination on the Electrochemical Activity and Double Layer Capacitance of Graphitic Carbons — *Lei Li, Haitao Liu*

**12:45 Paper 515b:** Colloidal Electronic Cells Based on 2D Materials — *Pingwei Liu, Albert Tianxiang Liu, Daichi Kozawa, Juyao Dong, Volodymyr Koman, Max Saccone, Jingfan Yang, Song Wang, Youngwoo Son, Min Hao Wong, Michael Strano*

**1:00 Paper 515c:** One-Step Non-Destructive Decoration of Transition Metal Oxide Nanoparticles on Large Scale Graphene for Electronic and Sensing Applications — *Songwei Che, Sanjay Behura, Vikas Berry*

**1:15 Paper 515d:** Large-Scale Chemical Synthesis of Graphene for Energy Storage and Biological Applications — *Michael Bozlar*

**1:30 Paper 515e:** Achieving High Open-Circuit Voltage in Graphene/Silicon Photovoltaic Cells with h-BN Tunneling Layer — *Chen Wang, Vikas Berry, Sanjay Behura*

**1:45 Paper 515f:** Multicolumn Gel Chromatography for Scalable Separation of Nanosheets Based on Size and Surface Chemistry — *Dorsa Parviz, Michael Strano*



**2:00 Paper 515g:** Graphene Interfaced Geobacter for Improved Electron-Transport Channels in Microbial Fuel Cell: A Single Cell Investigation — **Sheldon Cotts, Bijentimala Keisham, Vikas Berry**

**2:15 Paper 515h:** Synthesis of Graphene from Biochar — **Rahul Kundu, Hema Ramsum**

**2:30 Paper 515i:** Stabilizing Phosphorene Via Hexagonal Boron Nitride Passivation — **Natechanok Yutthasakunthorn, Sanjay Behura, Vikas Berry**

## (516) Highly Selective Separations with Membranes I

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 304

Dibakar Bhattacharyya, Co-Chair  
Stephen Ritchie, Co-Chair

**Sponsored by:** Membrane-Based Separations

**12:30 Paper 516a:** High Speed Production of Graphene Oxide Membranes and Their Potential Usage in Harsh Environments — **Mainak Majumder**

**12:55 Paper 516b:** New Highly CO<sub>2</sub>-Selective Amine-Based Membranes for Carbon Capture — **Yang Han, Witopo Salim, Kai Chen, W.S. Winston Ho**

**1:20 Paper 516d:** Membranes for Charge- and Aromaticity-Based Separation of Small Molecules — **Ayşe Asatekin, Ilcin Sadeghi**

**1:45 Paper 516e:** Metal Organic Brush (MOB) Membranes for Organic Solvent Nanofiltration — **John J. Keating, Somdatta Bhattacharya, Georges Belfort**

**2:10 Paper 516f:** Pi Electron Cloud Mediated Separation of Aromatics Using Supported Ionic Liquid (SIL) Membrane Having Antibacterial Activity — **S. Ranil Wickramasinghe, Arijit Sengupta, M. G. Jebur, Mohanad Kamaz, Xianghong Qian**

**2:35 Paper 516g:** Removal and Recovery of Ammonia from Dilute Aqueous Process/Effluent Streams — **Philip Aligwe, Kamalesh K. Sirkar**

## (517) Immunotherapy Applications

**Wednesday, Oct 31, 12:30 PM**  
Westin Convention Center, Pennsylvania East

Yvonne Y. Chen, Chair  
Wilson Wong, Co-Chair

**Sponsored by:** Immunotherapy

**12:30 Paper 517a:** Fueling Cancer Immunotherapy through Metabolic Reprogramming — **Greg Delgoffe**

**1:05 Paper 517b:** Macrophage Checkpoint Blockade in a Cell-Based Immunotherapy Can Generate Durable and Safe Cures in a Poorly Immunogenic, Syngeneic Mouse Tumor Model — **Lawrence J. Dooling, Jason C. Andrechak, Cory Alvey, Dennis E. Discher**

**1:23 Paper 517c:** Development of a Kynureninase Clinical Candidate, a First-in-Class Enzymatic Checkpoint Inhibitor — **John Blazeck, Catrina Somody, Ahlam Qerqez, Kyle Ford, Kendra Garrison, Christos Karamitros, Everett Stone, George Georgiou**

**1:41 Break**

**1:48 Paper 517d:** Immunotherapeutic Targeting of Cancer Cell-Associated Polysialic Acid — **Emily C. Cox, Dana N. Thornlow, Michaela A. Jones, Matthew P. DeLisa**

**2:06 Paper 517e:** Novel Immunomodulatory Peptide Polymers for Vascularized Composite Allograft Rejection Prevention — **Xiaofei Wang, Rui Zhang, Dylan Weir, Caitlin Leeper, Andrew Greenwald, Bret Ulery**

**2:24 Paper 517f:** CO-Delivery of Paclitaxel and Imatinib By PEG Derivatized NLG Carrier As Enhanced Immunotherapy — **Jieni Xu**

## (518) Interfacial and Nonlinear Flows: Drops, Bubbles and Films

**Wednesday, Oct 31, 12:30 PM**  
Omni William Penn Hotel, Phipps

Robert H. Davis, Chair  
Hao Sun, Co-Chair

**Sponsored by:** Fluid Mechanics

**12:30 Paper 518a:** Computational Analysis of Pinch-Off Dynamics and Printability of Simple and Complex Fluids — **Jelena Dinic, Vivek Sharma**

**12:45 Paper 518b:** Three-Dimensional Surfactant-Covered Flows of Thin Liquid Films on Rotating Cylinders — **Weihsia Li, Satish Kumar**

**1:00 Paper 518c:** Tear Formation at the Unstable Receding Contact Line of an Evaporating Meniscus — **Monojit Chakraborty, Justin A. Weibel, Suresh V. Garimella**

**1:15 Paper 518d:** The Liquid Film Behavior Outside a Twin-Fluid Atomizer and the Model Prediction — **Yule Zhu, Yuxin Wu, Junfu Lv, Guoli Tang**

**1:30 Paper 518e:** Buckling of Thin Elastic Films Under Viscous Stress — **Sourav Chatterjee, Christina McDonald, Rui Huang, Sachin Velankar**

**1:45 Paper 518f:** Evaporation-Driven Solutocapillary Flow of Thin Liquid Films over Curved Substrates — **Eric S. G. Shaqfeh, Mariana Rodriguez-Hakim, Joseph M. Barakat, Xinyi Shi, Gerald G. Fuller**

**2:00 Paper 518g:** Breakup of a Drop Under a Stagnation Point Flow — **Alireza Hooshanginejad, Nikolas A. Wilkinson, Cari S. Dutcher, Michael J. Shelley, Sungyon Lee**

**2:15 Paper 518h:** Electrostatic Faraday Instability in Thin Films — **Dipin Pillai, Ranga Narayanan**

**2:30 Paper 518i:** Parametric Study on Factors Affecting Bubble Dynamics during the Immersion Frying Process — **Shreya Sahasrabudhe, Brian Farkas**

**2:45 Paper 518j:** The Shape Evolution of Droplets in Miscible Environments — **Dan Walls, Eckart Meiburg, Gerald G. Fuller**

## (519) Membranes for Bioseparations

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 301

Heather C. S. Chenette, Chair  
Stephen M. Ritchie, Co-Chair

**Sponsored by:** Bio Separations

**12:30 Paper 519a:** Polymeric Microparticles as a New Platform for High Removal of Lipopolysaccharides — **Sidharth Razdan, Sutapa Barua**

**12:50 Paper 519b:** Lignocellulosic Materials for Nanofiltration Membrane Synthesis — **Andrew Colburn, D. Bhattacharyya**

**1:10 Break**

**1:30 Paper 519d:** Purification of Scfv Via Small Molecule Based Affinity Membrane Spin Column — **Franklin Mejia, Nur Mustafaoglu, Michael Canonico, Maura Vrabel, Basar Bilgicer**

**1:50 Paper 519e:** New Protein A and Multimodal Anion-Exchange Membranes for the Rapid Isolation and Purification of Biologics — **Daniel Henn, Jinxing Zhou, Scott M. Husson, Anna Forsyth, Graham Temples**

**2:10 Paper 519f:** Virus Filtration: Effect of Protein Fouling and Transmembrane Pressure — **Fatemeh Fallahianbajan, Sal Giglia, Christina Carbrello, Andrew L. Zydney**

**2:30 Paper 519g:** Process Optimization of Constant Flow Series Filtration of Bioprocess Fluids — **Sal Giglia, Sherry Ashby Leon**

## (520) Molecular Simulation of Adsorption I

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 305

Alexander Neimark, Chair  
Ateeque Malani, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**12:30 Paper 520a:** Understanding the Unique Sorption of Alkane- $\alpha,\omega$ -Diols in All-Silica Zeolites — **Robert F. DeJaco, Bahman Elyassi, Matheus Dorneles de Mello, Nitish Mittal, Michael Tsapatsis, J. Ilja Siepmann**

**12:50 Paper 520b:** A New Approach to Predict Adsorption in Metal-Organic Frameworks with Unsaturated Metal Sites — **Christopher Campbell, Kristina Sladekova, Michael Fischer, José R. B. Gomes, Miguel Jorge**

**1:10 Paper 520c:** The Effect of Intrinsic Framework Flexibility on Adsorption Properties in Metal-Organic Frameworks: A Computational Exploration — **Mayank Agrawal, Dai Tang, David S. Sholl**

**1:30 Paper 520d:** Quasi-2D Phase Transition of Methane Adsorbed in Cylindrical Silica Mesopores — **Daniel W. Siderius, William P. Krekelberg, Wei-Shan Chiang, Vincent K. Shen, Yun Liu**

**1:50 Paper 520e:** Molecular Model Development with Reliable Charge Distributions for Gaseous Adsorption in Nanoporous Materials — **Eun Hyun Cho, Li-Chiang Lin**

**2:10 Paper 520f:** Computational Design of Electric Field Responsive Metal-Organic Frameworks for Directional Flow — **Sadanandam Namsani, Benjamin Tam, Ozgur Yazaydin**

**2:30 Paper 520g:** Temperature Dependence of the Elastic Moduli of Confined Liquid Argon — **Christopher D. Dobrzanski, Gennady Gor**

**(521) Multiscale and Coarse-Grained Modeling of Polymers****Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 326

Jian Qin, Chair  
Douglas Tree, Co-Chair**Sponsored by:** Polymers**12:30 Paper 521a:** Structure and Dynamics in Sulfonated Polyphenylenes from Atomistic and Coarse-Grained Simulations — **Amalie L. Frischknecht****1:00 Paper 521b:** Developing Chemically Specific Coarse-Grained Conjugated Polymer Models Using the Taffi Framework — **Brett Savoie****1:15 Paper 521c:** Accessing Phase Behavior of Block Copolymer Grafted Nanoparticles Using Coarse-Grained Simulations and Protracted Colored Noise Dynamics — **Andrew Peters****1:30 Paper 521d:** Mesoscale Modeling of Polymer Solutions Under Flow — **Michael P. Howard, Antonia Statt, Arash Nikoubashman, Athanassios Z. Panagiotopoulos****1:45 Paper 521e:** Formation, Stability, and Annihilation of a “Stitch” Morphology in Block Copolymer Thin Films — **Cody Bezik, Juan J. de Pablo****2:00 Paper 521f:** Coarse-Grained Molecular Simulation Studies of Melting Thermodynamics of Oligonucleic Acids Conjugated with Polymers — **Prhashanna Ammu, Arthi Jayaraman****2:15 Paper 521g:** Versatile Hybrid Particle-Field Approach for Simulating Inhomogeneous Polymeric Systems — **Dong Meng, Jing Zong****2:30 Paper 521h:** Systematic and Many-Chain-Simulation-Free Coarse Graining of Polymer Melts: Structure-Based Coarse Graining of the Kremer-Grest Model — **Yan Wang, Qiang (David) Wang****2:45 Paper 521i:** Small Ion Effects on Self-Coacervation Phenomena in Block Polyampholytes — **Scott P.O. Danielson, Kris Delaney, Glenn H. Fredrickson****(522) Multi-Scale Modeling****Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 405

Andrew J Adamczyk, Chair  
Hari Nair, Co-Chair  
Josh Allen, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**12:30 Paper 522a:** *Extracting Transport Independent Kinetics for Vapor Phase Upgrading of Biomass Pyrolysis Vapors over H-ZSM-5* — **Vivek Bharadwaj, Brennan Pecha, Anne Starace, Calvin Mukarakate, Peter N. Ciesielski****12:50 Paper 522c:** Resolved-Pore CFD Simulation of CO Oxidation in a Catalyst Layer — **Behnam Partopour, Anthony G. Dixon****1:10 Paper 522d:** Experiments and Modeling for Enhanced Transport in SCR and Ammonia Slip Catalysts — **Pritpal Singh Dhillon, Michael Harold, Ashok Kumar, Saurabh Y. Joshi, Di Wang****1:30 Paper 522e:** DFT and Microkinetic Modeling Study of Ethanol from Syngas on Co<sub>2</sub>Pd<sub>6</sub> Nanocluster — **Anuradha Gundamaraju****1:50 Paper 522f:** CFD Simulation of a Bench Scale Fixed Bed Fischer-Tropsch Synthesis Reactor — **Jianqi Shen, Xinying Liu, Wei Hua Ho, Diane Hildebrandt****2:10 Paper 522g:** Establishing Discrete Ising Model for Zeolite Deactivation: Inspiration from the Game of Go — **Dali Cai****(523) Nanomaterials for Hydrogen Production and Fuel Cells II****Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 412

Seung Soon Jang, Chair  
Doh C. Lee, Co-Chair**Sponsored by:** Nanomaterials for Applications in Energy and Biology**12:30 Paper 523a:** Porous Structure Based High Performance Electrocatalysts for Low Temperature Fuel Cells — **Jinwoo Lee****1:00 Paper 523b:** Hydrogen Generation Ability of Perovskite and Spinel Redox Materials Via Thermochemical Water Splitting — **Joseph Houck, Vinod S. Amar, Jibrán Mahadik, Rajesh Shende****1:20 Paper 523c:** Solution Combustion Synthesis of Ni-Pt/CeO<sub>2</sub> nanocomposites for Hydrogen Generation Using Catalytic Decomposition of Hydrous Hydrazine — **Eric Walter, Wooram Kang, Arvind Varma****1:40 Paper 523d:** Synthesis of Nitrogen and Sulfur Co-Doped Graphene on Graphite Foam for Enhanced Electrochemical Oxygen Evolution and Phenol Degradation — **Xiaomeng Guo, Xiaobin Fan, Guoliang Zhang, Fengbao Zhang, Yang Li, Wenchao Peng****2:00 Paper 523e:** Development of Cell Reversal Tolerant Anode Catalysts for Automotive Polymer Electrolyte Membrane Fuel Cell — **Chanho Pak, Seung Woo Lee, Ji Yeon Lee, Eunyung You****2:30 Paper 523f:** An Earth-Abundant Tungsten-Nickel Alloy Electrocatalyst for Superior Hydrogen Evolution — **Jean Marie Vianney Nsanzimana****2:50 Paper 523g:** One-Dimensional Earth-Abundant Based Nanomaterials As Oxygen Evolution Reaction Electrocatalysts for Acid Mediated Proton Exchange Membrane Based Water Electrolysis — **Shrinath Ghadge, Oleg Velikokhatnyi, Moni Datta, Prashant Kumta****(524) Nanoscale Phenomena in Macromolecular Systems****Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 327

Kenneth Mineart, Chair  
Chris Iacovella, Co-Chair**Sponsored by:** Polymers**12:30 Paper 524a:** Conformations of Weak Polyelectrolytes in Confined Geometries — **Jonathan K. Whitmer****1:00 Paper 524b:** Quantifying Structure-Function Relationships of Protein-Selective Networks at the Micro- and Macro-Scale — **John R. Clegg, Joann Gu, Abhijeet Venkataraman, Nicholas A. Peppas****1:15 Paper 524c:** Block Copolymer Directed Self-Assembly Using Chemoepitaxial Guiding Underlayers with Topography — **Peter J. Ludovice, Benjamin Nation, Clifford L. Henderson****1:30 Paper 524d:** A New Class of “Gecko Leg” Dendrimeric Polymeric Particles By Interfacial Templating of Multiphasic Liquids — **Sangchul Roh, Austin Williams, Orlin D. Velev****1:45 Paper 524e:** Effect of Asymmetric Homopolymer Addition on Structural Characteristic of Lamellae Forming Block Copolymers Aligned Via Directed Self-Assembly — **Caleb Breaux, Jakin B. Delony, Peter Ludovice, Clifford L. Henderson****2:00 Paper 524f:** Theory and Simulation Studies of Structure and Thermodynamics in Polymer Nanocomposites Containing Grafted Nanoparticles — **Arjita Kulshreshtha, Arthi Jayaraman****2:15 Paper 524g:** Computational Characterization of Ultrathin Amorphous Polymer Films in Liquids — **Qisong Xu, Jianwen Jiang****2:30 Paper 524h:** Photocrosslinking to Obtain Graphitic Carbon-Based Nanowires from Ordered Polymer Networks — **Alan Aguirre-Soto****2:45 Paper 524i:** Multi-Scale Simulations of the Fabrication of Polymeric Nanoparticles through Rapid Solvent Exchange — **Nannan Li, Arash Nikoubashman, Athanassios Z. Panagiotopoulos****(525) Nanotechnology for Biotechnology and Pharmaceuticals I****Wednesday, Oct 31, 12:30 PM**

David L. Lawrence Convention Center, 311

Kevin J. Cash, Chair  
Margaret Bennewitz, Co-Chair**Sponsored by:** Bionanotechnology**12:30 Paper 525a:** Invited Speaker: Scalable Manufacturing Methods for Polymeric Nanoparticle Drug Delivery Systems — **Jessica O. Winter****1:10 Paper 525b:** Optimization of Calcium Phosphate-Polymer Nanoparticle System for Co-Delivery of microRNA-21 Inhibitor and Doxorubicin — **Vishnu Sriram, Mina Jafari, Joo-Youp Lee****1:28 Paper 525c:** Nanoallergens: A Liposomal Diagnostic Platform for Platinum-Based Drug Allergies — **Baksun Kim, Peter Deak, Jaeho Shin, Tanyel Kiziltepe, Basar Bilgicer****1:46 Paper 525d:** A Novel Approach for the Synthesis of Metallic Nanoparticles on Top of a Tellurium Nanowire Using a Green Synthesis Approach for Biomedical Applications — **Ada Vernet Crua, David Medina, Thomas J. Webster**

**2:04 Paper 525e:** Formulation and Recovery of Fast-Acting Lumefantrine Nanoparticles for Oral Malaria Therapy — *Jie Feng, Yingyue Zhang, Simon A. McManus, Kurt D. Ristroph, Robert K. Prud'homme*

**2:22 Paper 525f:** Engineering Antibacterial Nanosurfaces for Field Hospitals — *James W. Moxley Jr., Paria Ghannadian, Thomas J. Webster*

**2:40 Paper 525g:** Overcome Drug Resistance of Cancer Cells By Confining, Perturbing and Analyzing Them in Nano-Liter Chambers One Cell at a Time — *Yapeng Su, Wei Wei, Lidia Robert, Min Xue, Antoni Ribas, James Heath*

#### (526) NSF Workshop I: Highlights from CBET

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 411

Ram B. Gupta, Chair  
Richard Dickinson, Co-Chair

**Sponsored by:** Career Guidance Committee Liaison

**12:30 Paper 526a:** Overview of Chemical, Bioengineering, Environmental, and Transport Systems Division (CBET) — *Richard Dickinson*

**12:55 Paper 526b:** Highlights of CBET Cluster on Chemical and Biochemical Systems — *Carole Read*

**1:15 Paper 526c:** Highlights of CBET Cluster on Bioengineering and Engineering Healthcare — *Steven Peretti*

**1:35 Paper 526d:** Highlights on CBET Cluster on Environmental Engineering and Sustainability — *Bruce Hamilton*

**1:55 Paper 526e:** Highlights of CBET Cluster on Transport, Thermal and Fluid Phenomena — *Susan Muller*

**2:15 Paper 526f:** Interactive Question and Answer Session with NSF Program Directors — *Carole Read, Steven Peretti, Bruce Hamilton, Susan Muller, T. J. Mountziaris*

#### (527) Nucleation and Growth I

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 302

Venkateswarlu Bhamidi, Chair  
Meenesh R. Singh, Co-Chair

**Sponsored by:** Crystallization and Evaporation

**12:30** Welcoming Remarks

**12:35 Paper 527a:** A Stochastic PBE-Model of Crystallisation Accounting for Nucleation, Growth, and Chemical Reaction — *Giovanni Maria Maggioni, Marco Mazzotti*

**12:55 Paper 527b:** Binding Coefficients during Condensation of Au and Mg at High Temperatures By Molecular Dynamics Simulations — *Eirini Goudeli, Huan Yang, Christopher J. Hogan Jr.*

**1:15 Paper 527d:** Crystal Growth Kinetics of Stable and Metastable Polymorphs of Piracetam in Organic Solvents — *Ake Rasmuson, Rodrigo Soto*

**1:35 Paper 527e:** Templating Colloidal Crystal Growth Using Chirped Surface Relief Gratings — *Russell Mahmood, Andrew Mettry, Andrew C. Hillier*

**1:55 Paper 527f:** Mechanistic Insights into the Process of Crystallization Using a Kinetic, Multiscale Model — *Anish V. Dighe, Meenesh R. Singh*

**2:15 Paper 527g:** Insight into the Role of Piperazine in the Thermodynamics and Nucleation Kinetic of Triethylenediamine - Methyl Tertiary Butyl Ether System — *Yufeng Quan, Yang Yang, Shijie Xu, Peipei Zhu, Shiyuan Liu, Lina Jia, Xiaoyue Tan, Junbo Gong*

#### (528) Omics and High-Throughput Technologies

**Wednesday, Oct 31, 12:30 PM**  
Westin Convention Center, Butler

Ryan Koppes, Chair  
Nicholas Graham, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**12:30 Paper 528a:** From Skin to Nervous System : Experimental and Bioinformatics Approaches Investigating Signaling in Neural Crest Stem Cells from Interfollicular Human Epidermis — *Georgios Tseropoulos, Samaneh moghadasi Boroujnei, Vivek K. Bajpai, Stelios T. Andreadis*

**12:48 Paper 528b:** Combined  $^2\text{H}$  and  $^{13}\text{C}$  Metabolic Flux Analysis Enables Novel Discoveries in *Zymomonas Mobilis* Metabolism Used for Renewable Biofuel Production — *Paul A. Adamczyk, Tyler B. Jacobson, Jennifer L. Reed, Daniel Amador-Noguez*

**1:06 Paper 528c:** An Efficient Omics Platform for the High-Throughput Identification of O- and N-Linked Glycans Attached to Diverse Proteins — *Kai Cheng, Gang Liu, Sriram Neelamegham*

**1:24 Paper 528d:** Imputation of Single-Cell Expression Data — *Nan Papili Gao, Rudiyanto Gunawan*

**1:42 Paper 528e:** Pathway-Based Analysis of the Liver Response to Intravenous Methylprednisolone (MPL) Administration in Rats: Acute Versus Chronic Dosing — *Alison Acevedo, Ana Berthel, Debra DuBois, Richard R. Almon, William J. Jusko, Ioannis P. Androulakis*

**2:00 Paper 528f:** Metabolomics Reveals That Inhibition of Nucleotide Synthesis Underlies Senescence of Human Mammary Epithelial Cells — *Alireza Delfarah, Sydney Parrish, Jesse Yang, Frances Seo, Si Li, Pin Wang, Nicholas A. Graham*

**2:18 Paper 528g:** Invited Speaker: Developing an Omics-Based Approach to Understand and Model Eukaryotic Signal Transduction — *Mark Marten, Cynthia Chelius, Liliane Ribeiro, Jyothi Kumar, Stephen Lincoln, Walker Huso, Ranjan Srivastava, Steven Harris*

#### (529) Particle Technology Awards Lectures (Invited Talks)

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 415

Bruce D. Hook, Co-Chair  
Rajesh Davé, Co-Chair

**Sponsored by:** Particle Technology Forum

**12:30** Introductory Remarks

**12:35 Paper 529a:** Particle Technology: From Fundamentals to Translational Pharmaceutical and Energy Applications — *Chi-Hwa Wang*

**1:15** Q&A

**1:25 Paper 529b:** Aerosol Particle Technology: from Carbon Black to Breath Sensors — *Sotiris E. Pratsinis*

**2:05** Q&A

**2:15 Paper 529c:** Towards Sustainable Energy and Materials: Carbon Capture and Conversion using Novel Liquid-like Nanoscale Hybrid Particulate Systems — *Ah-Hyung Alissa Park*

**2:55** Concluding Remarks

**(530) Planning and Scheduling I**  
**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 409

Pedro M. Castro, Chair  
Qi Zhang, Co-Chair

**Sponsored by:** Computers in Operations and Information Processing

**12:30 Paper 530a:** Scheduling with Preemption — *Pedro M. Castro, Iiro Harjunkoski, Ignacio E. Grossmann*

**12:49 Paper 530b:** Robust Planning and Scheduling for Processes with Equipment Degradation — *Johannes Wiebe, Ruth Misener*

**1:08 Paper 530c:** A Simultaneous Process Scheduling and Personnel Allocation Framework for Industrial-Scale Multipurpose Facilities — *Fernando Santos, Ricardo Fukasawa, Luis A. Ricardez-Sandoval*

**1:27 Paper 530d:** A Novel Mathematical Model for Short-Term and Medium-Term Scheduling of Multipurpose Batch Plants — *Nikolaos Rakovitis, Jie Li, Nan Zhang*

**1:46 Paper 530e:** An Algorithm Combining the Strengths of Discrete- and Continuous-Time Scheduling Models — *Hojae Lee, Christos T. Maravelias*

**2:05 Paper 530f:** Batch Scheduling with Quality-Based Changeovers — *Braulio Brunaud, Satyajith Amaran, Scott J. Bury, John M. Wassick, Ignacio E. Grossmann*

**2:24 Paper 530g:** A Computational Comparison of New Models for the Multi-Mode Resource Constrained Project Scheduling Problem with Optional Activities — *Nikolaos Lappas, Hua Wang, Chrysanthos E. Gounaris*

**2:43 Paper 530h:** Scheduling and Analytics – Towards Better Planning — *Iiro Harjunkoski*

#### (531) Polymer Processing and Rheology

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 333

Blair Kathryn Brettmann, Chair  
Keith M. Forward, Co-Chair

**Sponsored by:** Polymers

**12:30 Paper 531a:** Transforming Layered Materials into Mechanically-Robust Fibers and Hydrogels — *Alex M. Jordan, Kris Van de Voorde, LaShanda T.J. Korley*



**1:00 Paper 531b:** Designing PIM-1 Microfibers with Tunable Morphology and Porosity Via Controlling Solvent/Nonsolvent/Polymer Interactions — **Siyao Wang**, Gregory N. Parsons, Saad A. Khan

**1:15 Paper 531c:** Formation of Poly(*para*-phenylene) Fibers — **Burcin Ikizer**, Nese Orbey, Carl Lawton

**1:30 Paper 531d:** Particle Electrospinning of High Loading Fiber-Microparticle Composites — **Blair Kathryn Brettmann**

**1:45 Paper 531e:** Processing of Linear Low Density Polyethylene-Halloysite Nanotube (LLDPE/HNT) Nanocomposite at High Temperature Using a Two-Roll Calendaring Machine — **Bahareh Baheri**, Sunggyu Lee

**2:00 Paper 531f:** Extensional Relaxation Times of Dilute and Semi-Dilute Polymer Solutions — **Jelena Dinic**, Leidy N. Jimenez, Madeleine Biagioli, Vivek Sharma

**2:15 Paper 531g:** Iterative Modeling of Constraint Dynamics in Discrete Slip-Link Model — **Konstantin Taletskiy**, Jay D. Schieber

**2:30 Paper 531h:** Rheology of Polyelectrolyte Solutions: From Salt Effects to Applications — **Antonio Perazzo**, Emre Turkoz, Craig B. Arnold, Howard A. Stone

**2:45 Paper 531i:** Linear Viscoelasticity of Vitremer Melts: A Theoretical Understanding of Their Peculiar Rheological Behavior — **Ralm Ricarte**, Ludwik Leibler

### (532) Practical Applications of Computational Chemistry and Molecular Simulation

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 308

Michael Shirts, Chair  
Martin Sanborn, Co-Chair  
Jonathan Moore, Co-Chair  
Joseph Golab, Co-Chair  
Phillip R. Westmoreland, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**12:30 Paper 532a:** Are Modern Force Fields Sufficiently Reliable for Developing Fundamental Equations of State from Hybrid Data Sets? — **Richard A. Messerly**, Andrei Kazakov

**12:50 Paper 532b:** Competitive Binding of Ethylene, Water, and Carbon Monoxide in Metal-Organic Framework Materials with Open Cu Sites — **Wenqin You**, David S. Sholl, Yang Liu, Joshua D. Howe

**1:10 Paper 532c:** Thermal Transport in Interpenetrated Metal-Organic Frameworks — **Kutay Berk Sezginel**, Patrick Asinger, Hasan Babaei, Christopher E. Wilmer

**1:30 Break**

**1:50 Paper 532e:** QM and QM/MM Treatment of Ionic Liquid Binding to Cysteinated Porphyrin — **Atiya Banerjee**, Jindal K. Shah

**2:10 Paper 532f:** Computer-Aided Precursor Design and Process Development for Nanostructured Film Deposition — **Andrew J Adamczyk**

**2:30 Paper 532g:** Design of Biomaterials By Simulation and Experiment: Molecular Recognition, Assembly, and Applications — **Hendrik Heinz**

**2:45 Paper 532h:** Fully Automated Molecular Design with Atomic Resolution for Desired Properties — **Hsuan-Hao Hsu**, Chem-Hsuan Huang, **Shiang-Tai Lin**

### (533) Process Intensification through the Application of Microreactors, Multiphase Reactors, and Membrane Reactors

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 335

Jing Luo, Chair  
Matthaeus Siebenhofer, Co-Chair

**Sponsored by:** Process Intensification & Microprocess Engineering

**12:30 Paper 533a:** Particle Synthesis in Ultrasound-Integrated Microreactors — **Zhengya Dong**, Simon Kuhn

**12:55 Paper 533b:** Demonstration of Scale-out Methodology for Intensified Liquid-Liquid Processes — **Eduardo Garcíadiego Ortega**, Dimitrios Tsaoulidis, Panagiota Angeli

**1:20 Paper 533c:** Multiphase Microchannel Separation Utilizing Capillary Pressure Gradients — **Matthew Coblyn**, Conor Zobebelein, Goran Jovanovic

**1:45 Paper 533d:** Effect of Pressure on Ethane Dehydrogenation in MFI Zeolite Membrane Reactor — **Shailesh Dangwal**, Ruochen Liu, Savannah V Kirk, Seok-Jhin Kim

**2:10 Paper 533e:** Scaling a Micro Structured Reactor for Sugar Chemistry from Lab Via Pilot to Full Production Scale — **Manfred Kraut**, Georg Rabsch, Roland Dittmeyer

**2:35 Paper 533f:** Green Synthesis of Polyvinyl Butyral (PVB) Using Microreactor System and Recycling Technology — **Kai Wang**, Xiyan Lin, Baiyang Zhou, Guangsheng Luo

### (534) Process Modeling and Control Applications

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 408

David H. Gay, Chair  
Yu Yang, Co-Chair

**Sponsored by:** Systems and Process Control

**12:30 Paper 534a:** Designing Stochastic Model Predictive Control Based Neural Interface to Restore Communication between Brain Regions — **Joseph Schmalz**, Gautam Kumar

**12:49 Paper 534b:** Predictive Strategies for Control of Indoor Air Quality — **Hari S. Ganesh**, Hagen E. Fritz, Thomas F. Edgar, Attila Novoselac, Michael Baldea

**1:08 Paper 534c:** An Optimization-Based Feedback Control Strategy for Spatially-Uniform Dose Delivery Using Atmospheric Pressure Plasma Jets — **Dogan Gidon**, David B. Graves, Ali Mesbah

**1:27 Paper 534d:** Dynamic Real-Time Optimization of a Gas-Phase Polymerization Reactor — **Yajun Wang**, George S. Oostace, Rita A. Majewski, Lorenz T. Biegler

**1:46 Paper 534e:** Model Predictive Control of a Nonisothermal and Nonisobaric Membrane Reactor for Water-Gas Shift Reaction Applications — **Jacob Douglas**, Paul Akula, Gaurav Mirkar, Fernando V. Lima

**2:05 Paper 534f:** Operator-Triggered Advisory System for Electric Arc Furnace Process Optimization — **Smriti Shyamal**, Christopher L. E. Swartz

**2:24 Paper 534g:** Geosteering Using Image Logs and an Intelligent Bottomhole Assembly — **Jude Rodrigues**, Michael Nikolaou

**2:43 Paper 534h:** Intelligent Pressure Control Method for Managed Pressure Drilling — **Jeevan Dahal**, Oluwatosin Oyelakin, Banchao Shu, Isaac Snyder, Priyanka Shahi

### (535) Reaction Engineering for Biomass Conversion II

**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 401

Amrit Jalan, Chair  
Fernando Resende, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 535a:** Dual Functional Zr-KIT-5 Shows Remarkable Activity for Depolymerization of Corn Stover Lignin into Stable Phenolic Monomers — **Kakasaheb Nandiwale**, Andrew Danby, Anand Ramanathan, R. V. Chaudhari, Bala Subramaniam

**12:51 Paper 535b:** Reaction Condition Optimization for the Scalability of 1,4-Anhydroerythritol and Xylitol Conversion Via Heterogeneous ReO<sub>x</sub>-Pd/CeO<sub>2</sub> Catalysis — **Blake MacQueen**, Elizabeth Barrow, Jochen Lauterbach

**1:12 Paper 535c:** Selective Tuning of the Glycerol C-O Bond Cleavage Sequence on Copper-Modified Molybdenum Carbide Surfaces — **Zhexi Lin**, Weiming Wan, Salai C. Ammal, Kyung-Eun You, Andreas Heyden, Jingguang G. Chen

**1:33 Paper 535d:** Oxophilic Metal Oxide Modified Iridium Catalysts for Selective Production of Renewable Hydrocarbons — **Sibao Liu**, Basudeb Saha, Dionisios G. Vlachos

**1:54 Paper 535e:** Localizing Microwave Heat By Surface Polarization of Titanate Nanostructures for Enhanced Catalytic Reaction Efficiency — **Tuo Ji**, Jiahua Zhu

**2:15 Paper 535f:** Selective Glucose to Fructose Isomerization over Modified Zirconium UiO-66 in Alcohol Media — **Matheus Dorneles de Mello**, Michael Tsapatsis

**2:36 Paper 535g:** Production of Biorenewable Monomers - from Fructose to 2,5-Furandicarboxylic Acid — **Ali Hussain Motagamwala**, Wangyun Won, David Martin Alonso, Christos Maravelias, James A. Dumesic



### (536) Safety and Sustainability Best Practices

Wednesday, Oct 31, 12:30 PM

David L. Lawrence Convention Center, 315

William M. Barrett, Chair  
Konstantinos E. Kakosimos, Co-Chair

Sponsored by: General

**12:30 Paper 536a:** Application of Simplified LOPA and Development of Risk Matrix for a University or Small Operational Company — **Tomasz Olewski**

**12:55 Paper 536b:** Role of Academia in Educating Students and Industry Professionals in Process Safety: Experience from MKOPSC-Qatar — **Luc Vechot, Tomasz Olewski**

**1:20 Paper 536c:** Waste Management Enhancement Strategies Learned from Hurricane Harvey — **Jian Fang, Hao Luo, Helen Lou, Renzun Zhao, Danny Reible**

**1:45 Paper 536d:** The Future Is Here: Robotic Catalyst Removal - Field Results 2018 — **Christopher R. Jansen, Andrew W. Sloley, Scott Schroeder**

**2:10 Paper 536e:** Back from the Future: What Nanotechnology Risk Analysis Can Teach Us about Process Safety Today — **Kristen M. Kulinowski**

**2:35 Paper 536f:** Measuring Safety Decision-Making Effectiveness with an Engineering Process Safety Research Instrument (EPSRI) — **Matthew Cooper, Brittany Butler, Daniel Anastasio, Daniel D. Burkey, Cheryl A. Bodnar**

### (537) Sustainable Energy Generation and Utilization in System Design

Wednesday, Oct 31, 12:30 PM

David L. Lawrence Convention Center, 410

Dharik Mallapragada, Chair  
Kirti Yenkie, Co-Chair

Sponsored by: Systems and Process Design

**12:30 Paper 537a:** Addressing Uncertainty in Large-Scale Bioconversion Product and Process Networks with Two-Stage Adaptive Robust Optimization — **Daniel Garcia, Jian Gong, Fengqi You**

**12:49 Paper 537b:** A Flexible Design Framework for Process Systems with Demand Response Objectives — **Yu Liu, Nael H. El-Farra, Ahmet Palazoglu**

**1:27 Paper 537d:** Accounting for Uncertainty Via Scheduling Informed Optimal Design: A Renewable Ammonia Case Study — **Andrew Allman, Matthew J. Palys, Prodromos Daoutidis**

**1:46 Paper 537e:** Design and Optimization of Multifunctional Processes for Utilizing Unconventional and Distributed Feedstocks — **Akhil Arora, Ishan Bajaj, Shachit S. Iyer, M. M. Faruque Hasan**

**2:05 Paper 537g:** Simultaneous Process Synthesis and Heat Integration Using Building Block Superstructure — **Salih E. Demirel, Jianping Li, M. M. Faruque Hasan**

**2:24 Paper 537h:** Green Operation of an Air Separation Unit Using an Efficient MILP Optimal Scheduling Framework — **Morgan Kelley, Ross Baldick, Michael Baldea**

### (538) Synthesis and Assembly of Electronic and Photonic Materials

Wednesday, Oct 31, 12:30 PM

David L. Lawrence Convention Center, 330

Joshua Choi, Chair  
Piran Kidambi, Co-Chair

Sponsored by: Electronics and Photonics

**12:30 Paper 538a:** *Invited:* Quasi-Two-Dimensional Materials: Synthetic Challenges and Structure-Tunable Properties — **Rainie D. Nelson, Atefe Hadi, Utkarsh Ramesh, Yujie Wang, Matthew G. Panthani**

**1:00 Paper 538b:** Mechanisms for Controlled Dynamics in Gold Nanoparticle-DNA Origami Templates — **Abhilasha Dehankar, Joshua Johnson, Matthew Sheffield, Michael Poirier, Ezekiel Johnston-Halperin, Carlos E. Castro, Jessica O. Winter**

**1:15 Paper 538c:** Interfacial Carbene Reactions on Hard and Soft Material Interfaces — **Alexander Shestopalov**

**1:30 Paper 538d:** Photothermal Assembly and Modification of Nanomaterial Heterostructures — **Matthew Crane, Elena P. Pandres, E. James Davis, Vincent C. Holmberg, Peter Pauzaskie**

**1:45 Paper 538e:** A Machine Learning Approach to Identifying Polymorphs and the Molecular-Scale Mechanisms By Which They Interconvert in Small-Molecule Organic Semiconductors — **Nikita Sengar, Paulette Clancy**

**2:00 Paper 538f:** Revealing Governing Mechanism in Directed Self-Assembly of Sub 10 Nm Particles into Textured Substrates — **Zhen Luo, Shafiq Mehraeen**

**2:15 Paper 538g:** Angle-Independent Structural Colors from Colloidal Glasses — **Seung-Hyun Kim, Jongwook Ha, Vinodhan N. Manoharan, Gi-Ra Yi**

**2:30 Paper 538h:** Spontaneous out of Plane Growth of ReS<sub>2</sub> for Solar Energy Harvesting — **Debjit Ghoshal, Anthony Yoshimura, Tushar Gupta, Andrew House, Yanwen Chen, Tianmeng Wang, Sagnik Basuray, Sufe Shi, Nikhil Koratkar**

**2:45 Paper 538i:** Understanding Armchair Graphene Nanoribbon Growth on Mis-Cut Ge(001) Surfaces through Experiments and Density Functional Theory Calculations — **Ellen A. Murray, Robert M. Jacobberger, Florian Göttl, Austin J. Way, Michael S. Arnold, Manos Mavrikakis**

### (539) Tribute to Jacques L. Zakin: Scholar, Teacher and Mentor II (Invited Talks)

Wednesday, Oct 31, 12:30 PM

Omni William Penn Hotel, Conference Center A

Martin Feinberg, Chair  
Kurt W. Koelling, Co-Chair

Sponsored by: Interfacial Phenomena

**12:30 Paper 539a:** Molecular Design of Wormlike Surfactant Micelles – Effects of Branching — **Norman J. Wagner, Michelle A. Calabrese**

**1:00 Paper 539b:** Tuning Weak Intermolecular Forces to Tune Self Assembly and Rheology: Hydrophobically Modified polymers, Surfactants, and Cyclodextrins — **Robert K. Prud'homme**

**1:30 Paper 539c:** The Spreading and Shape Evolution of Ultra-low Surface Tension Droplets — **Gerald G. Fuller**

**2:00 Paper 539d:** Cargo Carrying Bacteria at Interfaces — **Kathleen J. Stebe**

**2:30 Paper 539e:** Mechanistic Constitutive Model for Wormlike Micelle Solutions with Flow-induced Structure Formation — **Michael D. Graham**

### (540) USA-China Progress in Biomass Conversion Technology II

Wednesday, Oct 31, 12:30 PM

David L. Lawrence Convention Center, 325

Bandaru V. Ramarao, Chair  
Xinshu Zhuang, Co-Chair

Sponsored by: Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**12:30 Paper 540a:** Comparative Analysis of Microalgae Productivity Potential and Economic Analysis in Open Raceway Ponds and Flat Panel Photobioreactors — **Sudhanya Banerjee, Shri Ramaswamy**

**12:50 Paper 540b:** Subcritical Extraction of *Chlorella Pyrenoidosa*: Optimization through Response Surface Methodology — **Selvakumar Thiruvendakam, Michael K. Danquah, Razif Harun**

**1:10 Paper 540c:** Lignin-Derived Deep Eutectic Solvents Pretreatment of Herbal Residues to Enhance Enzymatic Digestibility of Cellulose — **Qiang Yu, Long Chen, Xinshu Zhuang, Zhenhong Yuan**

**1:30 Paper 540d:** The Dehydration of Biomass-Derived Fructose into 5-Hydroxymethylfurfural over the Layered Solid Acids HTaMoO<sub>6</sub> and HTaMoO<sub>6</sub> Nanosheets Aggregates — **Lele Jin, Wenzhi Li**

**1:50 Paper 540e:** Analysis of the Topochemistry of Lignocellulosic Biomass and Modeling of the Reaction Dissolution Phenomena — **Christopher M. Thomas, Bandaru V. Ramarao, Sahana Ramanna, Shri Ramaswamy, Feng Xu**

### (541) Workshop: Teaching Design (Products, Processes, and Industry Involvement)

Wednesday, Oct 31, 12:30 PM

David L. Lawrence Convention Center, 413

Benjamin J. Davis, Chair

Sponsored by: Undergraduate Education

**12:30 Paper 541a:** Client-Sponsored and Team-Defined Senior Capstone Projects — **Lauren Anderson**

**12:52 Paper 541b:** Embedding Engineering Research in Process Design Education — **Daniel Christe, Matteo Caligaris**

**1:14 Paper 541c:** Effective PBL in Senior Design: Examples & Lessons — **Christiaan Richter**

1:08 Break

**1:36 Paper 541d:** Incorporating Laboratory Pilot Plant Data and Customized Software Simulations into Chemical Engineering Design Education at Vanderbilt — **Russell F. Dunn**, **Matt Lang**, **Bryan Beyer**

**1:58 Paper 541e:** Implementation of Joint Senior and First-Year Design Projects — **Kimberlyn Gray**

#### (542) Ammonia Combustion: Turbines, Furnaces, Engines

**Wednesday, Oct 31, 1:15 PM**  
David L. Lawrence Convention Center, 317

Trevor Brown, Co-Chair

**Sponsored by:** NH<sub>3</sub> Energy+

**1:15 Paper 542a:** Basic Co-Firing Characteristics of Ammonia with Pulverized Coal in a Single Burner Test Furnace — **Akira Yamamoto**, **Masayoshi Kimoto**, **Yasushi Ozawa**, **Saburo Hara**

**1:30 Paper 542b:** Development of Low-NO<sub>x</sub> Combustor of Micro Gas Turbine Firing Ammonia Gas — **Osamu Kurata**, **Norihiko Iki**, **Takahiro Inoue**, **Takayuki Matsunuma**, **Taku Tsujimura**, **Hirohide Furutani**, **Masato Kawano**, **Keisuke Arai**, **Ekenechukwu C. Okafor**, **Akihiro Hayakawa**, **Hideaki Kobayashi**

**1:45 Paper 542c:** Two Stage Ammonia Combustion in a Gas Turbine like Combustor for Simultaneous NO and Unburnt Ammonia Reductions — **Akihiro Hayakawa**, **K.D. Kunkuma A. Somarathne**, **Masaaki Tsukamoto**, **Taku Kudo**, **Hideaki Kobayashi**

**2:00 Paper 542d:** Simulation Analysis of NH<sub>3</sub> Mixed Combustion in Clinker Manufacturing Process — **Tatsuro Izumi**, **Hiroki Kujiraoka**, **Yuya Yoshizuru**, **Takeshi Suemasu**, **Makoto Ueda**, **Toyooki Niki**, **Takayasu Itou**, **Masayuki Nishio**, **Ryuichi Murai**, **Fumiteru Akamatsu**

**2:06 Paper 542e:** Optimization of the NO<sub>x</sub> Reduction Condition in the Combustion Furnace for the Combustion of "Heavy-Oil - NH<sub>3</sub> System" Using CFD — **Yuya Yoshizuru**, **Takeshi Suemasu**, **Masayuki Nishio**, **Ryuichi Murai**, **Fumiteru Akamatsu**

**2:12 Paper 542f:** Ignition of an Aqueous Ammonia/Ammonium Nitrate Fuel — **Bar Mosevitzky**, **Gennady E. Shter**, **Gideon S. Grader**

**2:18 Paper 542g:** Improved Method of Using Hydrogen and Ammonia Fuels for an Internal Combustion Engine — **David Toyne**, **Jay Schmucker**

**2:24 Question & Answer session:** Ammonia Combustion

**2:30 Paper 542h:** Auto-Ignition Kinetics of Ammonia at Intermediate Temperatures and High Pressures — **Xiaoyu He**, **David Nascimento**, **Bo Shu**, **Kai Moshhammer**, **Mario Costa**, **Ravi Fernandes**

**2:45 Paper 593b:** Experimental and Computational Study for Reduction of NO<sub>x</sub> Emissions in the Ammonia/Methane Co-Combustion in a 10 Kw Furnace — **Ryuichi Murai**, **Ryohei Omori**, **Yuya Yoshizuru**, **Takahiro Kitano**, **Hidetaka Higashino**, **Noriaki Nakatsuka**, **Jun Hayashi**, **Fumiteru Akamatsu**

**3:00 Paper 542j:** Realization of Compression Ignition Engine Using Ammonia As a Sole Fuel with New Combustion Strategy — **Hyun HO PARK**, **Han Ho Song**

#### (543) Sustainable Ammonia Synthesis: Electrochemical Production

**Wednesday, Oct 31, 1:15 PM**  
David L. Lawrence Convention Center, 318

Trevor Brown, Co-Chair

**Sponsored by:** NH<sub>3</sub> Energy+

**1:15 Paper 543a:** A Low Pressure Membrane Based Renewable Ammonia Synthesis — **Sarbjit Giddey**

**1:30 Paper 543b:** Identifying the Prospects of Electrochemical Ammonia Synthesis on Mxenes Using First Principles Calculations — **Gurjot Sethi**, **Venkatasubramanian Viswanathan**

**1:36 Paper 543c:** Highly-Selective Electrochemical Reduction of Dinitrogen to Ammonia at Ambient Temperature and Pressure — **Qiang Zhang**, **Xiaoyang Cui**, **Cheng Tang**

**1:42 Paper 543d:** Electrochemical Synthesis of Ammonia Using Metal Nitride Catalysts — **Jared Nash**, **Xuan Yang**, **Jacob Anibal**, **Yushan Yan**, **Bingjun Xu**

**1:48 Paper 543e:** Electrochemical Nitrogen Reduction Reaction on Transition Metal Nitride Nanoparticles in Proton Exchange Membrane Electrolyzers — **Xuan Yang**, **Jared Nash**, **Jacob Anibal**, **Marco Dunwell**, **Yushan Yan**, **Bingjun Xu**

**1:54 Question & Answer session:** Electrochemical I

**2:00 Paper 543f:** DFT Analysis of Elementary N<sub>2</sub> Electro-Reduction Kinetics on Transition Metal Surfaces — **Sharad Maheshwari**, **Gholamreza Rostamikia**, **Yawei Li**, **Lauren F. Greenlee**, **Julie N. Renner**, **Michael Janik**

**2:06 Paper 543g:** Enhanced Electrochemical Ammonia Production Via Peptide-Bound Metal — **Charles Loney**, **David Suttmitter**, **Lauren F. Greenlee**, **Michael J. Janik**, **Julie N. Renner**

**2:12 Paper 543h:** New Insights into Electrocatalysis of Nitrogen Reduction to Ammonia — **Alex Schechter**, **Revanasiddappa Manjunatha**

**2:18 Paper 543i:** Electrochemical Reduction of Nitrogen to Ammonia over Transition Metals — **Victoria Smith**, **Aditya Prajapati**, **Meenesh R. Singh**

**2:24 Question & Answer session:** Electrochemical II

**2:30 Paper 543n:** A Study on Electrochemical Ammonia Synthesis with Proton-Conducting Solid Oxide Electrolytic Cells Based on La<sub>0.8</sub>Sr<sub>0.2</sub>Gd<sub>0.8</sub>Mg<sub>0.2</sub>O<sub>3-δ</sub> — **Kangyong Lee**, **SeungJin Jeong**, **WooChul Jung**, **Joongmyeon Bae**

**2:36 Paper 543k:** Low-Pressure Electrolytic Ammonia Synthesis Via High-Temperature Polymer-Based Proton Exchange Membrane — **Ted Aulich**

**2:42 Paper 543l:** Atmonia: Sustainable Ammonia Production Using Electrocatalysis at Ambient Temperature and Pressure — **Helga Dagg Flosadottir**, **Egill Skúlason**, **Fatemeh Hanifpour**, **Arnar Sveinbjörnsson**, **Fríðrik Magnus**, **Younes Abghoui**, **Jian Yang**

**2:48 Paper 543m:** Electrochemical Synthesis of Ammonia Using Nitrogen and Water in Alkaline Electrolytes Under Ambient Conditions — **Shreya Mukherjee**, **Gang Wu**

**2:54 Question & Answer session:** Electrochemical III

**3:00 Paper 543o:** Analysis of Influence of Operating Pressure on Dynamic Behavior of Ammonia Production over Ruthenium Catalyst under High Pressure Condition — **Hideyuki Matsumoto**, **Javadi Rahat**, **Yuichi Manaka**, **Mika Ishii**, **Tetsuya Nanba**

**(544) Poster Session: Catalysis and Reaction Engineering (CRE) Division**  
**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

Iman Noshadi, Chair  
Andrew Teixeira, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**Paper 544a:** Kinetics of Palm Oil Ethanolysis — **Mario Andres Noriega**, **Paulo Cesar Narváez Rincón**, **Juan Guillermo Cadavid**

**Paper 544b:** Catalytic Conversion of Biomass to Value Added Chemicals and Fuels — **Amoolya Lalsare**, **Jianli Hu**

**Paper 544c:** Utilizing a DMSO-like Material in Presence of Sulfuric Acid for Selective Fructose to 5-Hydroxymethylfurfural Reaction in Water — **Mariah Whitaker**, **Nicholas Brunelli**

**Paper 544d:** Controlled Synthesis of Pt-Sn/Al<sub>2</sub>O<sub>3</sub> catalysts and Their Application in the Hydrodeoxygenation of Bio-Based Succinic Acid — **Patrick Howe**, **Joshua Gopeesingh**, **Jesse Q. Bond**

**Paper 544e:** Liquid-Liquid Microfluidic Flows for the Reactive Extraction of HMF — **Pierre Desir**, **Basudeb Saha**, **Dionisios G. Vlachos**

**Paper 544f:** Acid Hydrolysis of Glycosidic Bonds in Linear Polysaccharides from Food Waste: Kinetic Studies and Modeling — **Elvis Ebikade**, **Jonathan Lym**, **Basudeb Saha**, **Dionisios G. Vlachos**

**Paper 544g:** A Spectroscopic Study on the Glucose and Fructose Mutarotation Reactions in the Presence of Lewis and Brønsted Homogeneous Acids — **Athanasios Kritikos**, **Siddharth Panditrao**, **Pranav Ramesh**, **George Tsilomelekis**

**Paper 544h:** A Fundamental Study of Cellulose Hydrolysis in Super Acidic Molten Salt Hydrate Media — **Natalia Rodriguez Quiroz**, **Dionisios G. Vlachos**

**Paper 544i:** Conversion of Kraft Lignin to Value Added Aromatic Based Chemicals — **Deepak Raikwar**, **Saptarshi Majumdar**, **Debaprasad Shee**

**Paper 544j:** Unraveling Surface State and Composition of Highly Selective Nanocrystalline Ni-Cu Alloy Catalysts for Hydrodeoxygenation of HMF — **Jing Luo**, **Matteo Monai**, **Cong Wang**, **Jennifer Lee**, **Tomáš Duchoň**, **Filip Dvořák**, **Vladimír Matolín**, **Christopher Murray**, **Paolo Fornasiero**, **Raymond J. Gorte**

**Paper 544k:** Hydrotreating of Biomass Derived Bio-Oil/Bio-Crude — **Huamin Wang, Daniel Santosa**

**Paper 544l:** Transesterification of Waste Cooking Oil for Biodiesel Production Using Lithium Metasilicate Prepared from Fumed Silica — **Dai-Ying Lin, Bing-Hung Chen**

**Paper 544m:** Modeling Solvation Effects for Deoxygenation Reactions — **Neeraj Rai, Varsha Jain, Shanmuga Venkatesan, Woodrow Wilson, Jordyn Polito**

**Paper 544n:** Kinetic of the Esterification of Fatty Acids with Methanol for Biodiesel Production — **Dario Moreno, Andres Abril, Anderson Imbach, Luis Miguel Serrano Bermúdez, Camilo Monroy-Peña, Carlos A M Riascos, Paulo Cesar Narváez Rincón, Gustavo Buitrago**

**Paper 544o:** Understanding Catalytic Bifunctionality of Cu/ZSM5 and Cu/Y Zeolites for Biomass Conversions — **Jiayi Xu, Quanxing Zheng, Keith L. Hohn, Bin Liu**

**Paper 544p:** Rapid and Simultaneous Production of Furfural and Cellulose-Rich Residue from Sugarcane Bagasse Using a Pressurized Phosphoric Acid-Acetone-Water System — **Qiong Wang**

**Paper 544q:** Analysis of Hydrothermal Liquefaction of Food Waste into Biofuel and Biomaterials — **Aersi Aierzhati, Yuanhui Zhang, Michael Stablein**

**Paper 544r:** Fast Pyrolysis of Oil Palm Empty Fruit Bunch (EFB) into Bio-Oil for Transportation Fuel — **Rozzeta Dolah, Rohit Karnik, Halimatun Hamdan, Haryanti Yahaya**

**Paper 544t:** Corncob Residue As a Valuable Resource for the Production of Aromatics — **Yunfei Bai, Yongdan Li**

**Paper 544u:** MoO<sub>3</sub>-Catalyzed Conversion of Guaiacol into Alkylphenols in Supercritical Ethanol — **Zewei Ma, Yongdan Li**

**Paper 544v:** Catalytic Glycosylation of Glucose with Fatty Alcohol over Sulfonated Mesoporous Carbons — **Wahiba Ramdani, Ayman Karam, Karine Vigier, Sébastien Rio, Anne Ponchel, Francois Jerome**

**Paper 544x:** Thermo-Catalytic Conversion of Lignocellulosic Biomass to Levoglucosenone and 5-Chloromethyl Furfural in Fluidized Bed Reactor — **Anurag Parihar, Gil Garnier, Sankar Bhattacharya**

**Paper 544y:** Mechanocatalytic Depolymerization of Cellulose with Perfluorinated Sulfonic Acid Ionomers — **Prince N. Amaniampong, Ayman Karam, Karine Vigier, Francois Jerome**

**Paper 544z:** Pt-Ru/CNTs Electrocatalysts for Direct Methanol Fuel Cell — **Bahareh Alsadat Tavakoli Mehrabadi, John R. Regalbut, John Weidner, John R. Monnier**

**Paper 544aa:** Cheap and Upscalable Process for Atomic Layer Deposition on Powder through Stoichiometric Grafting in Solution — **Benjamin P. Le Monnier, Frederick Wells, Jeremy S. Luterbacher**

**Paper 544ab:** Automated Microfluidic Platform for High-Throughput Screening of Rhodium-Catalyzed Hydroformylation — **Cheng Zhu, Keshav Raghuvanshi, Connor W. Coley, Milad Abolhasani**

**Paper 544ac:** Atomic-Level Insight into Oxygen Adsorption on (hkl) Platinum Surfaces and Implications for the Reactivity in the Oxygen Reduction Reaction — **Shiyi Wang, Enbo Zhu, Yu Huang, Hendrik Heinz**

**Paper 544ad:** Immobilized Group IV Metal Precursors on Acidic Supports for Ethylene Oligomerization — **Joshua D. Wright, Galiya Magazova, Thomas F. Degnan, Jason C. Hicks**

**Paper 544af:** CO<sub>2</sub>-Triggered Recoverable Metal Nanocatalysts Using Unimolecular Core-Shell Star Copolymers As Carriers — **Yuchen Zhang, Pingwei Liu, Bo-Geng Li, Wen-Jun Wang**

**Paper 544ag:** Continuous Ligand-Free Palladium-Mediated Carbon-Carbon Cross-Coupling — **Jeffrey A. Bennett, Jan Genzer, Milad Abolhasani**

**Paper 544ah:** Simultaneous Cell Disruption and Semi-Quantitative Activity Assays for High-Throughput Screening of Thermostable L-Asparaginases — **Xian Zhang Sr., Taowei Yang Sr., Meijuan Xu, Zhiming Rao Sr., Shang-Tian Yang**

**Paper 544ai:** *In Situ* observation of Cu<sub>2</sub>O Island Reductive Shrinking on Cu(100) Facet Under Methanol Using Environmental Transmission Electron Microscopy — **Hao Chi, Christopher L. Andolina, Matthew Corman, Meng Li, Goetz Vesper, Judith C. Yang**

**Paper 544ak:** Thermodynamic Complexity of Sulfated Zirconia Catalyst — **Naiwang Liu, Li Shi, Di Wu, Alexandra Navrotsky**

**Paper 544am:** The Influence of Size and Surface Structure of Co<sub>3</sub>O<sub>4</sub>-Supported Pd Nano-Particles on CO Oxidation Activity — **Rui Huang, Kyeounghak Kim, Jeong Woo Han**

**Paper 544an:** Novel *in Situ* Methods to Resolve the Complex Pathways of Zeolite Crystal Growth Towards the Optimization of Microporous Catalyst Synthesis — **Madhuresh K. Choudhary, Manjesh Kumar, Rishabh Jain, Jeffrey D. Rimer**

**Paper 544ao:** Experimental Investigation of Bed Size Effects on the Hydrodynamics of Gas-Solid Fluidized Bed Reactor Via Advance Non-Invasive Measurement Techniques (CT and RPT) — **Abdelsalam Efhaima Sr., Muthanna H. Al-Dahhan**

**Paper 544ap:** Comparison between the Activities of Cu/Al<sub>2</sub>O<sub>3</sub> and TiO<sub>2</sub> in the Liquid Phase Oxidation of Methanol-Ethanol Mixtures: Development of a Kinetic Model for the Catalyst Preparation — **Francisco Jose Morales Leal, Javier Rivera de La Rosa, Carlos Javier Lucio Ortiz, Diana Bustos Martinez, David Alejandro de Haro del Rio, Marco Antonio Garza Navarro, Daniela Xulu Vargas Martinez, Carlos D Garcia**

**Paper 544aq:** First Principles Study of Active Sites on High Performance PGM-Free ORR Catalyst — **Gurjyot Sethi, Venkatasubramanian Viswanathan**

**Paper 544ar:** Investigation of Molecular Properties of Imidazolium-Based Ionic Liquids in the Presence of Cysteine Ligated Iron Porphyrins for Understanding Their Biodegradability — **Atiya Banerjee, Jindal K. Shah**

**Paper 544as:** Defect Engineering and Sulfation of MOF-808: Towards the Obtainment of Microporous-Mesoporous Structures with Strong Brønsted Sites for Catalysis Applications — **Carolina Ardila-Suárez, Victor Baldovino-Medrano, Gustavo Ramirez-Caballero**

**Paper 544at:** Prediction of Surface Energies for Complex Pt Structures from Coordination Number and Generalized Coordination Number — **Wen Zhong, Christopher L. Hanselman, Kevin Tran, Chrysanthos E. Gounaris, Zachary Ulissi**

**Paper 544au:** Understanding the pH Dependence of Reversible Hydrogen Reactions — **Saad Intikhab, Joshua Snyder, Maureen H. Tang**

**Paper 544ax:** Yolk-Shell Nanoparticle Functionalization for Heterogeneous Hydroamination — **Trent R. Graham, Ellis Hammond-Pereira, Andika Rosul, Steven R. Saunders**

**Paper 544ay:** Exploiting Pore Diffusion in Core@Shell Nanocatalysts — **Yahui Yang, Götz Vesper**

**Paper 544az:** The Effect of Inert Pellet Size in the Fixed-Bed Reactor for Fischer-Tropsch Synthesis — **Gi Hoon Hong, Young Su Noh, Ali Alizade Eslami, Hyun Dong Kim, Hyun-tae Song, Dong Ju Moon**

**Paper 544ba:** Bifunctional Zeolite-Encapsulated Pt Catalysts for Tandem Aldol Condensation and Hydrogenation of Furfural with Acetone — **Hong Je Cho, Bingjun Xu**

**Paper 544bb:** Developing First-Principles Based Embedded Atom Method Potentials for Metal Clusters Using Bayesian Statistics — **Noushin Omidvar, Siwen Wang, Hongliang Xin**

**Paper 544bd:** Carbon Sphere Supported Cobalt Catalysts for Fischer Tropsch Synthesis — **Mahluli Moyo**

**Paper 544be:** Zirconium Hydroxide-Based Sorptive and Catalytic Textiles — **Natalie Pomerantz, Erin Anderson, Nick Dugan, Nicole Hoffman, Joe Rossin, Rachel Rossin, Pearl Yip**

**Paper 544bf:** Synthesis of Nanoporous Zeolite-Y Assisted By an Inexpensive Bifunctional Cationic Polymeric Template — **Aasif Dabbawala, Yasser Al Wahedi, Marios Katsiotis, Balasubramanian Vaithilingam, Stephane Morin, Mikael Berthod, Gnana Pragasam Singaravel, Saeed Alhassan**

**Paper 544bg:** Simple and Cost-Effective Treatment to Enhance Hydrophobicity of Zeolites — **Aamena Parulkar, Nitish Deshpande, Nicholas Brunelli**

**Paper 544bh:** Criteria for a Unique Steady State for Guava Juice Depectinization in a Continuous Stirred Tank Reactor — **Sourav Sengupta, Sirshendu De**

**Paper 544bi:** Theoretical Investigation of the Effects of Metal Cations on Oxygen Reduction Reaction in Non-Aqueous Metal-Air Batteries — **Saurin Rawal, William C. McKee, Ye Xu**

**Paper 544bj:** Exploring ORR Activity at the Organic/Metal Interfaces — **Megha Anand, Samira Siahrostami, Jens Norskov**



**Paper 544bl:** Electrodeposited Co-Mo-TiO<sub>2</sub> Composites for the Hydrogen Evolution Reaction — **Cheng Wang**, Elizabeth J. Podlaha-Murphy

**Paper 544bm:** Metal Supported Ultrathin Oxide/Oxyhydroxide Thin Films for Oxygen Reduction Reaction — **Seoin Back**, Samira Siahrostami, Michal Bajdich, Jens Norskov

**Paper 544bn:** Electrodeposited Fe-Rich, Fe-Ni-Co Thin Films for Oxygen Evolution Reaction — **Yujia Zhang**, Elizabeth J. Podlaha-Murphy

**Paper 544bo:** Dual CO Light-Off Effect on Pt/Al<sub>2</sub>O<sub>3</sub>, Pd/Al<sub>2</sub>O<sub>3</sub>, Pt/CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and Pd/CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> in the Presence of C<sub>3</sub>H<sub>6</sub> — **Rudolf Pecinka**, Jan Brezina, Marek Vaclavik, Petr Koci

**Paper 544bp:** Addressing Electronic Conductivity Limitations in Non-Precious Metal Alloy Electrocatalysts — **Rituja Patil**, Aayush Mantri, James R. McKone

**Paper 544bq:** Dual Role of Surfactants in Zeolite Catalyst Synthesis and Optimization — **Aseem Chawla**, Rui Li, Rishabh Jain, R. John Clark, James Sutjianto, Jeremy Palmer, Javier García-Martínez, Jeffrey D. Rimer

**Paper 544br:** Supported Perovskite Oxides for Low Temperature CO<sub>2</sub> Conversion By Reverse Water-Gas Shift Chemical Looping — **Bryan J. Hare**, Debanu Maiti, Yolanda A. Daza, Adela E. Ramos, Venkat R. Bhethanabotla, John N. Kuhn

**Paper 544bs:** Tuning Parameters for Tertiary Amine Catalysts Grafted on Mesoporous Silica for Knoevenagel Condensation — **Ashwin Kane**, Nitish Deshpande, Aamena Parulkar, Mariah Whitaker, Rutuja Joshi, Pinaki Ranadive, Nicholas Brunelli

**Paper 544bt:** The Role of Hydroxyl Groups in Carbon Monoxide Oxidation over Copper-Titanium Dioxide Catalysts — **Guoqiang Cao**, Nan Yi

**Paper 544bu:** Applications of Microwave Plasma Catalysis — **Ashley Caiola**, Sarojini Tiwari, Xinwei Bai, Amoolya Lalsare, Jianli Hu

**Paper 544bv:** A Facile Approach to Prepare Pt Nanoclusters Encapsulated within the Micropores of Zeolite — **Lisa Nguyen**, Junjun Shan, Hui Wang, Jihong Cheng, John Matsubu, Yizhi Xiang, Fu-Kuo Chiang

**Paper 544bw:** Mechanistic Insights into the Role of Zr Dopants in Ceria Based Ketone Catalysts — **Ashutosh Mishra**, Craig L. Perkins, Allison Robinson, Vassili Vorotnikov, J. Will Medlin, Eric M. Karp

**Paper 544bx:** Stability of Fe and Zn Promoted Mo/ZSM-5 Catalysts for Ethane Dehydroaromatization in Cyclic Operation Mode — **Brandon Robinson**, Xinwei Bai, Victor Abdelsayed, Dushyant Shekhawat, Jianli Hu

**Paper 544bz:** The Use of Iron Ore As Fischer Tropsch Synthesis Catalyst — **Katuchero Ramutsindela**

**Paper 544ca:** Single Rhodium and Palladium Atoms Anchored in Micropores for Transformation of Methane to Acetic Acid and Methanol Under Mild Condition — **Franklin (Feng) Tao**, Yu Tang, Victor Fung, De-en Jiang

**Paper 544cb:** Synthesis, Characterization, and Application of Ruthenium-Doped SrTiO<sub>3</sub> Perovskite Catalysts for Microwave-Assisted Methane Dry Reforming — **Lalit Gangurde**

**Paper 544cc:** Porous Titania Microspheres: Highly-Efficient Catalyst Scaffold for Green Syngas Production — **Matthew Parker**, Zachary Campbell, Jacob Lustik, Daniel Jackson, Seif Yusuf, Fanxing Li, Milad Abolhasani

**Paper 544cd:** Controlled Post-Synthesis Modification Enables Tuning of ZSM-11 Catalyst Performance in the Methanol-to-Hydrocarbon Reaction — **Thuy T. Le**, Heng Dai, Jeffrey D. Rimer

**Paper 544ce:** Adding Water to the Feed of Formic Acid Decomposition over  $\alpha$ -MoC Catalyst on Graphite — **Yahya Aldoshan**, Su Ha, Jake T Gray

**Paper 544cf:** Platinum Vs. Ruthenium: A Kinetic Comparison of Vapor-Phase Acetone Hydrogenation — **Xin Gao**, Omar A. Abdelrahman, Jesse Q. Bond

**Paper 544cg:** Different Catalytic Behaviors of Pd and Pt Metals in Decalin Dehydrogenation to Naphthalene — **Kyeounghak Kim**, Jeong Woo Han

**Paper 544ch:** Exploring the Effect of Chloride-Ion Exposure on CN, and Fe-N-C Catalysts for Application As Oxygen Depolarized Cathodes in Chlorine Production — **Deeksha Jain**, Kuldeep Mamtani, Vance Gustin, Seval Gunduz, Anne Co, Umit S. Ozkan

**Paper 544ci:** Surfactant-Templated MOF — 808: Effect of CTAB Incorporation on Final Properties and Catalytic Activity — **Carolina Ardila-Suárez**, Iván Mora-Vergara, Victor Baldovino-Medrano, Gustavo Ramírez-Caballero

**Paper 544cj:** Diffusion of Light Gases in Nanoporous Gold By Pulsed Field Gradient NMR — **Amineh Baniani**, Evan M. Forman, Marcus Bäumer, Sergey Vasenkov

**Paper 544ck:** Ice-Templating Fabrication of Hierarchical TS-1 Monoliths with Steam-Assisted Crystallization for Enhanced Benzene Hydroxylation — **Baoquan Zhang**, Luwei Geng, Xiufeng Liu

**Paper 544cl:** High-Performance Pt-Based Cathode Catalysts: Novel Carbon Supports and in-Situ Generation of Alloy Structure — **Mengjie Chen**, Gang Wu

**Paper 544cm:** Preparation of a SBA-15/Cordierite Monolith Support for Intensified Catalytic Reactions — **Thiago F. de Abreu**, Thiago L. R. Hower, Martin Schmal, Rita M. B. Alves

**Paper 544cn:** Mixed Metal Small Pore Zeolites: Synthesis, Characterization and Catalytic Testing — **Daniel F. Shantz**, Aibolat Koishybay

**Paper 544co:** One Preparation Method of High Aluminium-Content Sulfated Zirconia: The Influence of Aluminum Contents and Washing on the Structural Morphology, Acidity and Reactivity — **Zhiming Ma**, Li Shi

**Paper 544cp:** Iron Supported on Clinoptilolite (natural zeolites) As a Low-Temperature Fischer-Tropsch Synthesis Catalyst — **Roick Chikati**, Diakanua Nkazi

**Paper 544cq:** Imidazolium Based Porous Hypercrosslinked Ionic Polymers for Efficient CO<sub>2</sub> Capture and Fixation with Epoxides — **Jing Li**, Jiahua Zhu, Jun Wang

**Paper 544cr:** Synthesis of Novel Hierarchically Porous ZSM-5-KIT-5 Materials and the Catalytic Performances for Hydrodenitrogenation of Quinoline — **Qian Meng**, Aijun Duan, Cong Liu, Di Hu

**Paper 544cs:** Facile Fabrication of Dendritic Mesoporous Silica/Carbon Nanospheres for Selective Adsorptive Desulfurization — **Cong Liu**, Pei Yuan, Meng Qian, Hu Di, Aijun Duan

**Paper 544ct:** Controllable Synthesis of Spherical Al-SBA-16 Mesoporous Materials with Different Crystal Sizes and Its High Isomerization Performance for Hydrodesulfurization — **Hu Di**, Aijun Duan, Liu Cong, Meng Qian

**Paper 544cv:** Pore Size Effect on the Hydrogenation of Diesters over Ordered Hierarchical Cu/HPS Catalyst — **Yujun Zhao**, Bo Peng, Yue Wang, Shengping Wang, Xinbin Ma

**Paper 544cw:** Preparation of Highly Dispersed Iron Species over ZSM-5 with Enhanced Metal-Support Interaction By Freeze-Drying Impregnation — **Lisong Fan**, Dangguo Cheng, Fengqiu Chen, Xiaoli Zhan

**Paper 544cx:** Controllable Fabrication and Catalytic Performance of Nanosheet HZSM-5 Films By Vertical Secondary Growth — **Yajie Tian**, Li Wang, Qingfa Wang, Xiangwen Zhang, Guozhu Liu

**Paper 544cy:** Suitability of Developing Zeolite Y Catalyst from Ediko Nigeria Clay — **Esio Obobo**, Rasheed Babalola, Etim Bassey

**Paper 544cz:** Reaction Conversion of Gases in Plasma Reactors — **Joseph Toth III**, Xiaozhou Shen, Daniel J. Lacks, R. Mohan Sankaran

**Paper 544da:** Effect of Fe, Mg, Mo, and Pt Promoters on Ni-Based Catalysts over Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> for Oxidative Dehydrogenation of Methane with Carbon Oxide — **Abbas Jawad**

**Paper 544db:** Investigating the Effect of Addition of Potassium to the Mo/HZSM-5 during the Non-Oxidative Conversion of Methane to Aromatics — **Vaidheeswar Ramasubramanian**, Hema Ramsum, Geoffrey Price

**Paper 544dc:** Achieving Low-Cost and Accelerated Living Cationic Polymerization of Isobutyl Vinyl Ether in Microflow System — **DAN Xie**, Lu Yangcheng

**Paper 544hl:** Spectroscopic Insights into the Oxidation of Nitric Oxide over [Cu, Zn]-ZSM-5 — **Zachary T. Gentle**, Dan Shantz

**Paper 544hm:** Catalytic Hydrogenation of Carbon Monoxide to Formaldehyde in Functionalized Metal Organic Frameworks: An Investigation of Pathway — **Sen Zhang**, Lin Li, Jonathan Ruffley, J. Karl Johnson

**Paper 544dd:** Benchmarks for CO and CO<sub>2</sub> Adsorption on MnO(100): A Comparison of DFT to Experimental Data — **Han Chen**, Xu Feng, David F. Cox

**Paper 544de:** Theoretical Investigation of the Decomposition of Cyclohexane on Ir and Pt Surfaces — **Kushal Ghale**, Ye Xu

**Paper 544df:** Using Density Functional Theory Calculations to Probe the Activity of Brønsted Acid Sites in Zeolite — **Michael Zeets**, Bin Wang

**Paper 544dg:** A Fundamental Understanding of the Surface and Catalytic Chemistry of Transition Metal Ceramics in Deoxygenation — **Yang He, Siris Laursen**

**Paper 544dh:** Screening Bimetallic Catalyst for CO<sub>2</sub> Reduction Using Machine Learning and DFT Data — **Zong Qian Yu**

**Paper 544di:** Development of an Automatic Catalyst Evaluation System Controlled By a Spreadsheet Software — **Miyu Hirohara, Ken-Ichiro Sotowa, Toshihide Horikawa, Jesus Rafael Alcantara-Avila**

**Paper 544dj:** Theoretical Investigation of CO Adsorption and Disproportionation on Mo<sub>2</sub>C Nanotube Supported Pt Nanoparticles — **Zongtang Fang, Lucun Wang, M. Ross Kunz, Shuai Tan, Dongmei (Katie) Li, Ember Sikorski, Lan Li, Rebecca Fushimi, Gregory S. Yablonsky**

**Paper 544dk:** First-Principles Study of Hydrogen Dissociation on Plutonium Hydride — **Ryan Gotchy Mullen, Nir Goldman**

**Paper 544dl:** Robust Uncertainty Quantification Framework in Computational Electrochemical Functional Materials Design — **Venkatasubramanian Viswanathan, Dilip Krishnamurthy, Vaidish Sumaria**

**Paper 544dm:** Metal-Oxide Supported Pt Catalysts for Oxygen Reduction Reaction: A Density Functional Theory Approach — **Olga Vinogradova, Dilip Krishnamurthy, Lin Li, Venkatasubramanian Viswanathan**

**Paper 544dn:** Modelling of Four Phase Continuous Hydrogenation Systems — **Muzammil Khan, Sunil Joshi**

**Paper 544do:** High Throughput Alloy Catalysis across Composition Space — **Nicholas Golio, Irem Sen**

**Paper 544dp:** Experimental and Modeling Study to Investigate Optimized Washcoat Structure for Ammonia Slip Catalyst (ASC) — **Pritpal Singh Dhillon, Michael Harold, Ashok Kumar, Saurabh Y. Joshi, Di Wang**

**Paper 544dq:** Thermodynamic and Kinetic Analysis of  $\gamma$ -Valerolactone Ring Opening in Multiphase Reactors — **Xinlei Huang, Zijian Wang, Jesse Q. Bond**

**Paper 544dr:** Bayesian Chemisorption Theory of Catalysis — **Siwen Wang, Hongliang Xin**

**Paper 544ds:** Using Data Science to Reduce Large Reaction Networks in Catalysis — **Aini Palizhati, Zachary Ulissi**

**Paper 544dt:** Effect of Water, pH and Electrochemical Potential on Cl Adsorption on Cr<sub>2</sub>O<sub>3</sub> Passive Film — **Kofi Oware Sarfo, Pratik V. Markute, Zavalsa Quezada Gerardo, O. Burkan Isgor, Yongfeng Zhang, Julie D. Tucker, Liney Arnadottir**

**Paper 544du:** The Effect of Solvents on the Decomposition of Acetic Acid Using Density Functional Theory and Ambient Pressure XPS — **Sean Seekins, Kingsley Chukwu, Liney Arnadottir**

**Paper 544dv:** Density Functional Theory Study of Decarboxylation and Decarbonylation of Acetic Acid over Pd (111) — **Sean Seekins, Kingsley Chukwu, Liney Arnadottir**

**Paper 544dw:** The Use of Thermodynamics to Predict Cobalt Catalyst Speciation during Fischer Tropsch Reduction and Reaction — **Joshua Gorimbo, Diane Hildebrandt**

**Paper 544dx:** Influence of Salt on Nanozeolite-Y Particles Size Synthesized Under Organic Template Free Condition — **Hanin Radman, Asif Dabbawala, Yasser Al Wahedi, Gnana Pragasam Singaravel, Stephanie Morin, Mikael Berthod, Saeed Alhassan**

**Paper 544dy:** Thermodynamics of Sorption in Polyolefins in Gaseous and Liquid Media — **Martina Podivinská, Lenka Krajakova, Jaromir Ponedec, Juraj Kosek**

**Paper 544dz:** Modeling the Kinetics of Ethane Oxidative Dehydrogenation Via Chemical Looping — **Vasudev Pralhad Haribal, Luke Neal, Phillip R. Westmoreland, Fanxing Li**

**Paper 544ea:** Evaluation of the Benefits of Kinetic Monte Carlo and Microkinetic Modeling for Catalyst Design Studies in the Presence of Lateral Interactions — **Xiao Li, Lars C. Grabow**

**Paper 544eb:** Exploring Biocatalyst Design and Process Optimization Using Active Learning and Atomistic Simulations — **Ashraf Ali, Andrew J Adamczyk**

**Paper 544ec:** Theoretical Studies on the Gas-Phase Synthesis and Properties of Semiconducting Nanomaterials — **Yeseul Choi, Andrew J Adamczyk**

**Paper 544ed:** Analysis of Kinetics in the Ring-Opening Reaction and Decarboxylation of  $\gamma$ -Valerolactone and Pentenoic Acids over Zeolite Catalysts — **Xinlei Huang, Jesse Q. Bond**

**Paper 544ee:** Kinetic Assessments of the Location and Proximity of Brønsted Acid Sites in MFI Zeolites Containing Boron and Aluminum Heteroatoms — **Philip M. Kester, Elizabeth E. Bickel, Jeffrey T. Miller, Rajamani Gounder**

**Paper 544ef:** Equilibrium Analysis of Methylbenzene Intermediates for a Methanol-to-Olefins Process — **Dali Cai**

**Paper 544eh:** Computational and Experimental Investigations of Electrochemical CO<sub>2</sub> Reduction on a Well-Defined Model Surface — **Haochen Zhang, Mu-Jeng Cheng, Qi Lu**

**Paper 544ei:** A Machine Learning Model for Accelerating Biomimetic Electrocatalyst Discovery — **Hemanth S. Pillai, Noushin Omidvar, Junwei Luo, Hongliang Xin**

**Paper 544ej:** One Dimensional (1D) Earth-Abundant Based Nanomaterials As Oxygen Evolution Reaction Electrocatalysts for Acid Mediated Proton Exchange Membrane Based Water Electrolysis — **Shrinath Ghadge, Oleg Velikokhatnyi, Moni Kanchan Datta, Prashant Kumta**

**Paper 544ho:** Multivariate Analysis of Biomass Conversion Over Ruthenium Catalyst — **Xiaoping Chen, Jong-Min Lee**

**Paper 544ek:** Oxidative Desulfurization of Diesel Fuel Using Vanadium Supported Catalyst on Titanium Nanotube — **Navid Ranjbar, Mohammad Reza Dehghani, Farhad Banisharif**

**Paper 544el:** CO Oxidation By Single-Atom Pt Catalyst Anchored to Ni-Doped MgO — **Debolina Misra, Satyesh Yadav**

**Paper 544em:** Rapid Cycling to Achieve High NO<sub>x</sub> Conversion on Pt/CeO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> — **Zhiyu Zhou, Michael Harold, Dan Luss**

**Paper 544en:** Effect of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> supported Co and Fe Catalysts on Synthesis of Ammonia from CH<sub>4</sub> and N<sub>2</sub> Using Microwave Plasma — **Sarojini Tiwari, Xinwei Bai, Jianli Hu**

**Paper 544eo:** Effect of Different Metal Oxide Supported Cu Catalysts for 1,2-Propanediol Production Via Glycerol Hydrogenolysis Route — **Smita Mondal, Prakash Biswas**

**Paper 544ep:** Enhanced Stability of a Chromium Oxide on Alumina for Propane Dehydrogenation By Introduction of Cobalt — **Madhav Sethia, Nikita Dewangan, Hidayat Kus, Sibudjing Kawi**

**Paper 544eq:** Effects of Interface Adsorption of *Rhodococcus Ruber* TH3 Cells on the Biocatalytic Hydration of Acrylonitrile to Acrylamide — **Mingzhao Guo, Lufan Yang, Yujun Wang, Guangsheng Luo**

**Paper 544er:** Oxidative Desulfurization of Thiophenic Components By Vanadium Substituted Dawson-Type Polyoxometalate Supported Catalysts — **M Naderi Khomartaji, Mohammad Reza Dehghani, Farhad Banisharif**

**Paper 544es:** Quasi-2D Pd/Pt Nanoclams for CO<sub>2</sub> Reduction in Tandem with Microbial Communities — **Andrew B. Wong, Frauke Kracke, Antaeres Antoniu-Pablan, Alfred M. Spormann, Christopher Hahn, Thomas F. Jaramillo**

**Paper 544et:** Preparation of Ag-Doped TiO<sub>2</sub> Sol with Peroxo-Sol-Gel Method and Its Application on Antibacteria and Antivirus — **Yu-Wen Chen, Benjawan Moongraksathum**

**Paper 544eu:** Impact of Polymer-Based Protein Engineered  $\alpha$ -Chymotrypsin on Enantioselective Transesterification in Organic Media — **Hironobu Murata, Stefanie Baker, Yue Sun, Krzysztof Matyjaszewski, Alan Russell**

**Paper 544ev:** Direct Synthesis of Dimethyl Ether By CO<sub>2</sub> Hydrogenation over a High Active CuO/ZnO/ZrO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and HZSM-5 Bifunctional Catalyst — **Shoujie Ren, Weston R. Shoemaker, Xiaofeng Wang, Zeyu Shang, Naomi Klinghoffer, Shiguang Li, Miao Yu, Xinhua Liang**

**Paper 544ew:** Indirect Oxidation of Glucose to Glucuronic Acid Using Pd-Decorated Au Catalysts — **Yiyuan Yin, Li Chen, Z. Conrad Zhang, Michael S. Wong**

**Paper 544ex:** CO<sub>2</sub> Hydrogenation with Ni/MgO Catalysts — **Astrid Loder, Susanne Lux, Georg Baldauf-Sommerbauer, Matthaeus Siebenhofer**

**Paper 544ey:** Enhancement of Mo/ZSM-5 Catalysts in Methane Aromatization By Addition of Fe Promoters and By Reduction/Carburization Pretreatment — **Apoorva Sridhar**, Mustafizur Rahman, Sheima J. Khatib

**Paper 544ez:** Direct Conversion of Carbon Dioxide into Value-Added Chemicals — **Xinwen Guo**

**Paper 544fa:** The Production of H<sub>2</sub>-Rich Gas over SiC Modified Calcium-Aluminate Support Nickel Catalyst for Steam Reforming of Methane — **Young Su Noh**, Gi Hoon Hong, Ali Alizade Eslami, Hyun-tae Song, Seol A Shin, Hyun Dong Kim, Kwan-Young Lee, **Dong Ju Moon**

**Paper 544fb:** Non-Oxidative Direct Conversion of Methane over Fe(C)SiO<sub>2</sub> Catalyst with Controlling Radical-Based Reaction — **Seung Ju Han**, Yong Tae Kim

**Paper 544fc:** Exploring a Tandem Chemocatalytic Route from Syngas to Ethanol — **Marat Orazov**, David Chester Upham, Thomas F. Jaramillo

**Paper 544fd:** Dry-Reforming of Methane over M/Ni-M/Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub> (M = Pt, Fe, Mg, and Mo) Catalysts — **Abbas Jawad**, Fateme Rezaei, Ali Rowanaghi

**Paper 544fe:** Mechanistic Insights into the Prins Condensation of Formaldehyde with Butene Isomers over H-[Al]-ZSM5 Catalyst — **Sha Li**, Efterpi Vasiliadou, Raul F. Lobo, Dionisios Vlachos, Stavros Garatzoulas

**Paper 544ff:** Catalytic Reforming of Aqueous Methanol Using Double Cylinder Type Reactor — **Daisuke Kobayashi**, Mitsuyuki Hagiwara, Shin Kobayashi, Atsushi Shono, Yasukazu Saito

**Paper 544fg:** Molybdenum Enhanced the Catalytic Activity of Nickel Supported Alumina Catalyst for Hydrodeoxygenation of Stearic Acid — **Pankaj Kumar**

**Paper 544fh:** Methane Decomposition for the Production of CO<sub>x</sub>-Free Hydrogen and All Base Growth Carbon Nanotubes over Transition Metal Aerogel Catalysts — **Bingying Gao**

**Paper 544fi:** Studies on Fischer-Tropsch Synthesis over Co/Ru/Me-Apso-34 Catalyst — **Hyun Dong Kim**, Gi Hoon Hong, Ali Alizade Eslami, Young Su Noh, Hyun-tae Song, Ghaffari Saeidabad Nasim, **Dong Ju Moon**

**Paper 544fj:** Methane Decomposition for Carbon Nanotubes and CO<sub>x</sub>-Free H<sub>2</sub> over Fe-Based Catalysts on Different Supports — **I-Wen Wang**, Ayillath K. Deepa, Bingying Gao, Hanjing Tian, Jianli Hu

**Paper 544fk:** Temperature Programmed Surface Reaction and in-Situ IR Studies of the Oxidative Scission of Methyl Ketones over γ-Al<sub>2</sub>O<sub>3</sub> supported Vanadium Oxide — **Ran Zhu**, **Siwen Wang**, Jesse Q. Bond

**Paper 544fl:** Trireforming of Methane for the Production of Syngas over Fe@MWCNT/Co Catalysts — **Camila Emilia Figueira**, Martin Schmal, Reinaldo Giudici, Rita M. B. Alves

**Paper 544fm:** A Comparative Study of Nickel Impregnated ZrTiO<sub>2</sub> Catalysts for Hydrogen Gas Production Via Reforming of Methane — **Ali Alizade Eslami**, Seol A Shin, Hyun Dong Kim, Hyun-tae Song, Young Su Noh, Gi Hoon Hong, Ghaffari Saeidabad Nasim, **Dong Ju Moon**

**Paper 544fn:** Dehydroaromatization of Ethylene over Metal-ZSM-5 Catalysts — **Yunwen Zhou**, Ming-Feng Hsieh, Hari Thirumalai, Lars C. Grabow, Jeffrey D. Rimer

**Paper 544fp:** PtO<sub>x</sub> and PdO<sub>x</sub> Formation during NO Oxidation on Diesel Oxidation Catalysts — **Panagiotis Boutikos**, Adela Buzkova Arvajova, **Marek Vacilavik**, Petr Koci

**Paper 544fq:** Catalytic Activity of Magnetic Nanoparticles Activated Via RF Induction Heating — **Natalia da Silva Moura**, Pragathi Darapaneni, Kerry M. Dooley, **James A. Dorman**

**Paper 544fr:** Structure/Redox/Reactivity Properties of Dispersed Vanadium Species on TiO<sub>2</sub> for the Oxidative Dehydrogenation of Propane with CO<sub>2</sub> — **Hedun Wang**, George Tsilemelekis

**Paper 544fs:** Nanostructured Metal Nitrides and Carbides for Industrial & Environmental Catalysis — **Kenneth L. Roberts**

**Paper 544ft:** Hydrogenation of Phenol to Cyclohexanone Via Tubular Nanofiber Supported Catalyst — **Lin Pan**

**Paper 544fu:** Dimethyl Ether Synthesis from CO<sub>2</sub> Hydrogenation on a CuO-ZnO-Al<sub>2</sub>O<sub>3</sub>-CeO<sub>2</sub>/HZSM-5 Bifunctional Catalyst — **Yu-Wen Chen**

**Paper 544fv:** Oxidative Steam Reforming of Methanol over Cu-Zn-Al Oxides for the Production of Hydrogen — **Xiao Huang**, Shuirong Li, **Yun-Quan Liu**

**Paper 544fw:** Ni-Mo<sub>2</sub>C: A Highly Active Catalyst for Partial Oxidation of Jet Fuel — **Qusay Bkour**, M. Grant Norton, Su Ha

**Paper 544fx:** CO<sub>2</sub>-Free Hydrogen Production from Crude Oil through Microwave-Assisted Catalytic Deep Dehydrogenation — **Yuqiang Yan**, Sergio Gonzalez-Cortes, Benzheng Yao, Fahai Cao, Tiancun Xiao, Peter P. Edwards

**Paper 544fy:** Metal-Promoted Dehydroaromatization of Ethylene over ZSM-5 Catalysts — **Yunwen Zhou**, Ming-Feng Hsieh, Hari Thirumalai, Lars C. Grabow, Jeffrey D. Rimer

**Paper 544fz:** Decolouration of Dye Solutions By Oxidation with H<sub>2</sub>O<sub>2</sub> in the Presence of Modified Natural Zeolites — **Alina Korobeinyk**, Stavros Pouloupoulos, Aliya Sataeva, Aigerim Chinakulova, **Vassilis J. Inglezakis**

**Paper 544ga:** Oxidative Dehydrogenation of Propane to Propylene over VO<sub>x</sub>/CaO-γAl<sub>2</sub>O<sub>3</sub> — **Mohammad Mozahar Hossain**

**Paper 544gb:** Plasmonic Catalysts for Ammonia Synthesis — **Jessica Akemi Cimada da Silva**, Xiangkun Cao, David Erickson, Tobias Hanrath

**Paper 544hn:** Combined Capture and Utilization of CO<sub>2</sub> for Syngas Production over Dual-Function Materials — **Ahmed Al-Mamoori**, Ali Rowanaghi, Fateme Rezaei

**Paper 544gc:** Recent Developments in Designing Catalysts for Oxygen Reduction Reaction — **Samira Siahrostami**

**Paper 544gd:** Advanced Laser-Made Nanocatalysts for Solar Water Splitting — **Astrid M. Müller**

**Paper 544ge:** Synthesis and Applications of Heterogeneous Nitrides Nanophotocatalysts — **Prasaanth Ravi Anusuyadevi**, Cyril Aymonier, **Samuel Marre**

**Paper 544gf:** Tuning Cobalt and Nitrogen Co-Doped Carbon Nano Composites for Efficient Oxygen Reduction Reaction — **Mengran Liu**, **Yidong Liu**, Yong Min

**Paper 544gg:** Photocatalytic Degradation of Acid Violet 7 Dye Using a Composite of ZnO/Ppy in Annular Continuous Reactor — **Diego Alexander González Casamachin**, **Javier Rivera de La Rosa**, Carlos Javier Lucio Ortiz, Victor Manuel Ovando Medina, Nancy Elizabeth Davila-Guzman, David Alejandro de Haro del Rio, Diana Bustos Martínez, Gerardo Antonio Flores Escamilla, Francisco Jose Morales Leal

**Paper 544gh:** Degradation of Phenol By Heterogeneous Photocatalysis with TiO<sub>2</sub>-Modified BLACK MUD Catalysts — **Vitoria S. Lourenço**, **Yvan J. O. Asencios**

**Paper 544gi:** Electrochemical Charge Transfer Kinetics from Constrained Density Functional Theory — **Robert Warburton**, Márton Vörös, Larry Curtiss, Jeffrey Greeley

**Paper 544gj:** Combustion Synthesis of Ptzn Nanoparticle Electrocatalysts for Ethanol Oxidation in Alkaline Medium — **Md. Abdul Matin**, **Anand Kumar**

**Paper 544gk:** Electrochemical Conversion of Amines to Nitro Explosophores for Energetic Materials — **Brian F. Disalle**

**Paper 544gl:** Selective Electrochemical Reduction of CO<sub>2</sub> to Ethylene on Nanopores Modified Copper Electrodes in Aqueous Solution — **Yuecheng Peng**

**Paper 544gm:** Nanoporous Palladium Alloys As CO Poisoning Suppressing Electrocatalysts for Electrochemical Conversion of CO<sub>2</sub> to Formate — **Swarnendu Chatterjee**, Yawei Li, Joshua Snyder

**Paper 544gn:** Electroless Cu-Ni-Mo-P Catalyst for Electrooxidation and Thermochemical Oxidation of Glycerol — **Egwu E. Kalu**, Kayode F Adekunle, Oyidia Elendu, Ikenna J Nzeribe, Thaddeus Amaechi, Joel Sankar, Paul J Ezeani, Yaw D. Yeboah

**Paper 544go:** Enhancement of Photocatalytic Activity of Carbon Nitride By Hydrogen Peroxide Under Visible Light: A Closer Inspection on Reaction Intermediates — **Mathew M. Desipio**, Dipendu Saha

**Paper 544gp:** Single-Walled Carbon Nanotube Mediated in Situ Electrochemistry — **Albert Tianxiang Liu**, Yuichiro Kunai, Michael Strano



**Paper 544gq:** Effect of Lanthanum and Chlorine Doping on Strontium Titanates for the Electrocatalytically-Assisted Oxidative Dehydrogenation of Ethane — **Dhruba Jyoti Deka**, Doruk Dogu, Katja E. Binkley Meyer, Anshuman Fuller, Seval Gunduz, Nathaniel Kramer, Anne Co, Umit S. Ozkan

**Paper 544gr:** Catalytic Thiophene Oxidation By Groups 4 and 5 Zeolite BEA with  $H_2O_2$ : Mechanistic and Spectroscopic Evidence for the Effects of Metal Lewis Acidity and Solvent Lewis Basicity — **Daniel T. Bregante**, Ami Patel, Alayna Johnson, David W. Flaherty

**Paper 544gs:** Trends in Adsorption of Electro-Catalytic Water Splitting Intermediates on Hetero-Structures of Perovskite Oxides — **Liang Zhang**, Abhinav S. Raman, Aleksandra Vojvodic

**Paper 544gt:** Electrically Enhanced Catalytic Transfer Hydrogenation of Acetophenone in a Biphasic System — **Nan WANG**, Lawrence R. Weatherly

**Paper 544gu:** Improving Gasoline-Fed Solid Oxide Fuel Cell Performance with Nickel Catalyst Anode — **Qusay Bkour**

**Paper 544gv:** Carbonaceous Supports Decorated with Pt-TiO<sub>2</sub> Nanoparticles Using Electrostatic Self-Assembly Method As a Highly Visible Light Active Photocatalyst for CO<sub>2</sub> Photoreduction — **Afsanehsadat Larimi**

**Paper 544gw:** A Systematic Experimental Study on Electrochemical Oxidation of Methane over Transition Metals — **Aditya Prajapati**, Meenesh R. Singh

**Paper 544gx:** Kinetic Modelling of Simultaneous Photo-Catalytic Degradation of Phenolic Compounds and Reduction of Metal Ions with Nano-TiO<sub>2</sub> — **Aravind Satish**, Sharad M Sontakke, Anirban Roy

**Paper 544gy:** Electrode Engineering: Modifying the Hydrophilicity of Carbon Paper for Improved Cobalt Phosphide Hydrogen Evolution Catalysts — **Joel Sanchez**, Laurie A King, Thomas F. Jaramillo

**Paper 544gz:** Probing the (Photo) Electrochemical Stability of Atomic Layer Deposited Coatings for Solar-Driven Hydrogen Evolution — **David W. Palm**, Alexander DeAngelis, Nicolas Gaillard, Thomas F. Jaramillo

**Paper 544ha:** Insights into the Surface Chemical and Catalytic Properties of Photocatalysts That Dictate Activity and Product Distribution in CO<sub>2</sub> Photocatalytic Reduction By H<sub>2</sub>O — **Samiksha Poudyal**, Morghan Parker, Siris Laursen

**Paper 544hc:** Electrochemical Cycling Strategy for Selective C-C Bonded, Acetylene Production from CO<sub>2</sub> or CH<sub>4</sub> Using Water at Atmospheric Pressure — **Joshua M. McEnaney**, Brian A. Rohr, Adam Nielander, Aayush R. Singh, Jens K. Nørskov, Thomas F. Jaramillo

**Paper 544hd:** Nitrogen-Doped Carbon Nanostructures As Bifunctional Catalysts for Unitized Regenerative PEM Fuel Cells — **Deeksha Jain**, Kuldeep Mamtani, Anne Co, Umit S. Ozkan

**Paper 544he:** High Temperature Co-Electrolysis of CO<sub>2</sub> and H<sub>2</sub>O on La<sub>0.9-x</sub>Sr<sub>x</sub>Ni<sub>1-y</sub>Co<sub>2</sub>Fe<sub>1-y-z</sub>O<sub>3-δ</sub> Type Cathode Catalysts — **Dhruba Jyoti Deka**, Seval Gunduz, Taylor Fitzgerald, Anne Co, Umit S. Ozkan

**Paper 544hf:** Highly Durable Pt Fuel Cell Cathode Nanocatalysts Via Nitrogen, Manganese Co-Doped Carbon Derived from Polyaniline Hydrogel — **Zhi Qiao**, Gang Wu

**Paper 544hg:** Effects of Electrolyte Composition on Electrochemical CO<sub>2</sub> Reduction — **Joaquin Resasco**, Alexis T. Bell

**Paper 544hh:** Hierarchical, Titanium/Titania Electrocatalyst for Water Electrolysis — **Patricia Taboada-Serrano**, Xiang Li, Costas Tsouris

**Paper 544hi:** Interaction of Thiol Ligands with Gold and Its Effect on Electrocatalytic CO<sub>2</sub> Reduction — **Xun Cheng**, Yuxin Fang, John C. Flake, Ye Xu

**Paper 544hj:** Enhanced CO<sub>2</sub> Electroreduction to CH<sub>4</sub> and C<sub>2</sub>H<sub>4</sub> Via Selective Proton Transfer — **Marcel Schreier**, Yogesh Surendranath

**Paper 544hk:** High-Pressure Electrochemistry: The Electrochemical Reduction of Carbon Dioxide into Usable Fuels and Chemicals — **Austin McKee**, Alan Rassoolkhani, Jonathan Koonce, Abdulsattar Alsaedi, Wei Cheng, Syed Mubeen

## (545) Poster Session: Environmental Division

**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

Debalina Sengupta, Chair  
Sage R. Hiibel, Co-Chair  
Jeffrey Seay, Co-Chair  
Leslie M. Shor, Co-Chair

**Sponsored by:** Environmental Division

**Paper 545a:** Modeling and Experimental Approach Towards of Photoelectrocatalytic Bacterial Inactivation of *E. coli* Using Vertically Aligned ZnO/CuI for Water Treatment — **Rimzhim Gupta**, Jayant Modak

**Paper 545b:** Optimization and Green Synthesis (*Delonix regia* mediated) of Zero Valent Iron Nanoparticles — **Mausumi Mukhopadhyay**, Niraj Kulkarni, Preeti Dauthal

**Paper 545c:** A Statistical Investigation of Chinese Opinions on Environmental and Economic Sustainability — **Frederick Qiu**, Ethan Wang, Matthew Fan, Zuyi (Jacky) Huang

**Paper 545d:** Activation of Persulfates by Catalytic Nickel Nanoparticles Supported on N-doped Carbon Nanofibers for Degradation of Organic Pollutants in Water — **Yunjin Yao**, Jie Zhang, Mengxue Gao, Maojing Yu, Yi Hu, Zhuoran Cheng, Shaobin Wang

**Paper 545e:** Synthesis and Characterization of Nitrogen-Doped Sr<sub>4</sub>Nb<sub>2</sub>O<sub>9</sub> by Mechanochemical Method — **Kokoro Hirokawa**, Junichi Ida, Tatsushi Matsuyama

**Paper 545f:** Effect of Power Frequency on Various Organic Compounds (VOCs) Decomposition Using Nonthermal Plasma Reactor Combined with Ceramic Filter — **Tsubasa Eto**, Junichi Ida, Tatsushi Matsuyama, Hideo Yamamoto

**Paper 545g:** Fluorescent Metal Nanosensors in IR Range for Nitrate Detection in Water — **Mahdi Mohammadzadeh**, Holly A. Stretz, Richard Mu

**Paper 545h:** Carbon Capture and Utilization Using Metal Cation in Seawater-Based Wastewater — **Dongwoo Kang**, Yunsung Yoo, Jinwon Park

**Paper 545i:** Sustainability Assessment By Emergy Approach: Gold Mining Extraction in Colombia — **Natalia Andrea Cano**, Hector Ivan Velasquez Arredondo

**Paper 545j:** Investigation on CO<sub>2</sub> Capture and Utilization Using Simulated Bio-Gas and Extracted Metal Cations — **Yunsung Yoo**, Dongwoo Kang, Injun Kim, Jinwon Park

**Paper 545k:** Selective Lithium Recovery from Brine Using Li<sub>1-x</sub>Ni<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> /Ag Battery System — **Chosel P. Lawagon**, Grace M. Nisola, Rey Eliseo C. Torrejos, Seong-Poong Lee, Wook-Jin Chung

**Paper 545l:** Environmental Impacts of Pavement Rejuvenators — **John Bergendahl**, Joshua Anderson, Jacqueline Barr, Daniel Cammarata, Rachel Rivera, Christian Walck, Justin Waters

**Paper 545m:** Microencapsulated Fluorescent Gold for Ppb-Level Chromium(VI) Sensing — **Yiyuan Yin**, Christian L. Coonrod, Kimberly N. Heck, Michael S. Wong

**Paper 545n:** Benzene Methylation Catalysed By Hierarchically Porous Zeolite: An Effective Way to Promote Xylene Selectivity and Catalyst Lifetime for Large Scale Commercial Use — **Xuan He**, Xuedong Zhu

**Paper 545o:** Catalytic Removal of Polybrominated Diphenyl Ethers (PBDEs) in Effluent Gas from Thermal Desorption Treated Soils — **Feiyue Fan**, Long Zhao, Hong Hou

**Paper 545p:** Fluoride Removal By Geopolymeric Adsorbent Synthesized from LD Slag — **Chayan Sarkar**, Amar Nath Samanta, Jayanta Kumar Basu

**Paper 545q:** Identification and Enzymatic Characterization of a Novel NADH Dependent Azoreductase, Encoded By Azok in *Klebsiella pneumoniae* — **Shweta Dixit**, Sanjeev Garg

**Paper 545s:** Multi-Stage Hydrothermal Processing of Algae for Enhancing Biocrude Quality and Denitrogenation — **Umakanta Jena**, S. Kent Hoekman

**Paper 545t:** Ca<sub>3</sub>M<sub>2</sub>O<sub>7</sub> Solid Sorbents for CO<sub>2</sub> Capture: An in Situ X-Ray Diffraction Study — **Ehsan Hassani**, Tae-Sik Oh

**Paper 545u:** Effect of Aerosol on MEA Slip in Capturing Carbon Dioxide — **Ching-Hung Cheng**, Jia-Lin Kang, De-Hao Tsai, David Shan-Hill Wong, Shi-Shang Jang, Chung-Sung Tan

**Paper 545v:** Kinetics and Mass Transfer Performance of CO<sub>2</sub> Absorption into DEEA/MAE Solution — **Zhiwu Liang**, Hongxia Gao

**Paper 545w:** Vertical Gardening As Means for Sustainable FOOD Production in FOOD Insecure Urban Communities — **Dr. Robert W. Peters, Dr. Lee Moradi, Julia Ashlyn Manzella**

**Paper 545x:** Adsorption Modeling for CO<sub>2</sub> Capture in Water Stable MOFs — **Mohammed S. Ba-Shammakh**

**Paper 545y:** Modeling a Water Wash Sieve Tray for Aerosols Scavenging Using Computational Fluid Dynamics — **Siao-Han Huang, Jia-Lin Kang, Abhay Zambare, David Shan-Hill Wong, Shi-Shang Jang**

**Paper 545z:** The Production of Ammonium Sulfate from Sulfur Dioxide By the Desulfurization of a Flue Gas Using Aqueous Hydrogen Peroxide and Ammonium Solution — **Mohammed Alkhalidi**

**Paper 545aa:** Assessment of Carbon BIO-Fixation By MIXED Indigenous Microalgae — **Fares Almomani**

**Paper 545ab:** Fluid Flow and Nutrient Retention in Biochar Amended Soils — **Yi Chen, Kyriacos Zygourakis**

**Paper 545ac:** Sorption Characteristics of Nitrogen and Phosphorus Onto Biochar from Aqueous Solution — **Shamim Begum, Qwanikwia Hicklen, Taylor Crocker, AHM Golam Hyder, Ben Oni**

**Paper 545ad:** Lead Removal from Water Using Insoluble Bacterial Carboxymethyl Cellulose — **Ezequiel Rossi, Úrsula Montoya Rojo, Patricia Cerrutti, María Laura Foresti, María Inés Errea**

**Paper 545ae:** Design of an Electrochemical Cell for Desalination of Seawater — **Aditya Prajapati, Emily C. Yolo, Meenesh R. Singh**

**Paper 545af:** An Investigation of Flow Obstructions to Minimize Media Loss in Simultaneous Air/Water Backwash Operations in Gray Water Filtration Systems — **Migjen Istrefi, Sean Seik, Zenaída Otero Gephardt**

**Paper 545ag:** Application of Polysaccharide Derivatives As Novel Draw Solutes in Forward Osmosis for Protein Concentration — **Chun Ding, Yan Wang**

**Paper 545ah:** Analysis and Control of Al Concentration in Groundwater Based on Mathematical Modeling and Laboratory Tests — **Daria Popugaeva, Ajay K. Ray, Konstantin Kreyman**

**Paper 545aj:** Development and Mechanism Study of a Cost Effective Piggery Wastewater Treatment System — **Jian Fang, Fanfan Liu, Zhiwen Nong, Chengyuan Su, Julia Lin, Shu Gao, Helen Lou, Renzun Zhao, Zhi Huang**

**Paper 545ak:** Modeling the Ionic Transport in an Electrodialysis Cell: Investigating the Impacts of Non-Ideal Solution Behavior in the Cell — **Soraya Honarparvar, Danny Reible, Chau-Chyun Chen**

**Paper 545al:** Modeling the Ion Transport and Adsorption in a Capacitive Deionization Cell — **Xin Zhang, Danny Reible**

**Paper 545am:** Using Methanotrophic Microalgae Coculture for Wastewater Treatment — **Nathan Roberts, Q. Peter He, Jin Wang**

**Paper 545an:** Silver/Silver Chloride Electrodes for Deionization — **Neda Seyedhassantehrani, James W. Palko**

**Paper 545ao:** Boron Removal By a Co-Precipitation Method with Formation of Ettringite-like Compounds — **Yamasaki Akihiro, Miyuki Noguchi, Tsubasa Shimizu**

**Paper 545ap:** Feasibility of H<sub>2</sub>O<sub>2</sub> Production at Graphite Cathode Using Quantum Chemical Calculations — **Anam Asghar, Abdul Aziz Abdul Raman, Wan Mohd Ashri Bin Wan Daud**

**Paper 545aq:** Application of Biosurfactant Surfactin for Efficient Oil Separation from Waste Crude Oil Via Two-Step Process — **Xuwei Long, Ziyun Yang, Yungqiao Zu, Mingjie Jin**

**Paper 545ar:** Impact of Seasonal Salinity Variations in Estuarine Systems: Thermodynamic Feasibility Analysis of Pressure Retarded Osmosis (PRO) and Reverse Osmosis (RO) Combinations — **Arijit Chakraborty, Anirban Roy**

**Paper 545as:** Detection of Metallic Ions in Solution Using Optical Emission Spectroscopy of Plasma Driven By Bipolar Pulsed Power Sources — **Ching-Yu Wang, Cheng-Che (Jerry) Hsu**

**Paper 545at:** Iron(III)-Based Metal Organic Frameworks As Heterogeneous Fenton-like Catalysts for Organic Pollutants Degradation — **Xie Quan**

**Paper 545au:** Novel Materials and System Architecture for Membrane Based Water Treatment Technology — **Abdulsattar Alsaedi**

**Paper 545av:** Developing a Prototype: "Portable" Solution for "Potable" Water — **Ridhish Kumar, Shubham Lanjewar, Sudeep Nadukkandy, Anirban Roy**

**Paper 545aw:** Technoeconomic Optimization of Emerging Technologies for Regulatory Analysis: NH<sub>4</sub>HCO<sub>3</sub> Forward Osmosis for Power Plant Wastewater Treatment — **Daniel Gingerich, Timothy Bartholomew, Meagan Mauter**

#### (546) Poster Session: Fuels and Petrochemicals Division Wednesday, Oct 31, 3:30 PM

David L. Lawrence Convention Center, Exhibit Hall B

Chau-Chyun Chen, Chair  
Paul M. Mathias, Co-Chair  
Samira Abedi, Co-Chair

**Sponsored by:** Fuels and Petrochemicals Division

**Paper 546a:** Prediction of the Flash Points of Multicomponent Systems: Applications to Solvent Blends, Gasoline, Diesel, Biofuels and Jet Fuels — **Patrice Paricaud, Laurent Catoire**

**Paper 546b:** Assessment of Cloud Point Depression and Solid Phase Behavior of Fatty Acid Ethyl Esters in the Presence of 3-Methylbutyl Dodecanoate — **Maria D Robustillo Fuentes, Larissa C B A Bessa, Antonio J A Meirelles, Pedro A Pessoa Filho**

**Paper 546c:** Molecular Dynamics Simulation of Quaternary Ammonium Polycation Exchange Membrane Fuel Cell: Nanophase-Segregated Structure and Transport Properties — **Anna Harris, Seung Soon Jang**

**Paper 546d:** High-Resolution Differential Phase-Contrast (DPC) X-Ray Imaging for Multiphase Fluid Flow in Three-Dimensional Porous Media — **Maha Yusuf**

**Paper 546e:** Understanding Distillation Curves and Pseudocomponents — **Andrew W. Sloley**

**Paper 546f:** Design of Relief and Flare System for Liquefied Natural Gas Plant Using Dynamic Simulation — **Seung-Kwon Seo, Jaehyeon Yang, Chul-Jin Lee**

**Paper 546h:** Hydraulic Improvement of a Two-Phase Dehydration Unit for Heavy Crudes through CFD Simulation — **Francisco Lopez-Villarreal, Mayra Agustina Pantoja-Castro, Benjamín Portales-Martínez, Ángel Gómez González, José Manuel Domínguez-Esquivel**

**Paper 546i:** Modeling and Simulation of 1,3 Butadiene Production Process at Turndown Capacity — **Namit Tripathi, Srinivas Palanki, Qiang Xu**

**Paper 546j:** Soft Sensor Modeling of Methanol Concentration in the Methyl-Tert-Butyl Ether Production Process — **Fan Yang, Yang Liu**

**Paper 546k:** Simulation and Optimization of LNG Plant Hot Section — **Mohamed Hussein, Mary Katebah, Abdulla Al-Hajri, Easa Al-Musleh**

**Paper 546l:** Suitability of Alternative Aviation Fuels to Modern Aircraft: Impact of Fuel Composition on Liquid Phase Oxidation and Deposit Growth in Aircraft Fuel Systems — **Arij Ben Amara, Laurie Starck, Didier Pigeon, Martial Lepinay, Hervé Cleris, Bruno Galliot, Jean Christien, François Leblanc**

**Paper 546g:** Recent Advances and New Directions for Optimization of Production Scheduling in Crude-Oil Refineries — **Robert E. Franzoi Jr., Brenno C. Menezes, Jeffrey D. Kelly, Jorge A. W. Gut**

**Paper 300a:** Refinery-Wide Scheduling for Optimization of Multiple Unit-Operations in the Supply, Production, and Demand Chains in Fuels, Lubes, Asphalts and Petrochemicals Industries — **Robert E. Franzoi Jr., Brenno C. Menezes, Jeffrey D. Kelly, Jorge A. W. Gut**

**Paper 546m:** The Evaluation of Volatile Char Interaction by the Novel Designed Crucibles in TG — **Xiaoming Li, Jin Bai**

**Paper 546o:** Water Impact of a Gas Shale Production and Distribution System in Mexico — **Maria G Laguna-Martínez, Vicente Rico-Ramírez, José María Ponce-Ortega**

**Paper 546p:** Studies on the Oxidative Stability of Mineral Naphthenic Oils Using Commercial Antioxidants — **Antonio Pontes Filho, F. Murilo Luna, Célio L. Cavalcante Jr.**

**Paper 546q:** Enhancing Fracture Aperture and Evolution of New Fractures in Utica Shale By Subcritical Water Treatment — **Md. Rifat Hasan, M. Toufiq Reza**

**Paper 546r:** Utilization of *Omta Bimo* (*Kigelia pinnata*) peels As Economic Biobriquette for Community in Cepu District, Indonesia with Sni-01-6235-2000 As Quality Standard — **Meli Yulyana, Muhammad Agung Wahyudi, Muhammad Nur Hidayat**

**Paper 546z:** A Technoeconomic Analysis of the Chloralkali Process for Hydrogen Production Using Solar Energy — *Marisol Contreras, Syed Mubeen, Charles O. Stanier*

**Paper 546s:** Modification of ZSM-5 zeolite based additive in FCC process for maximizing propylene production — *Mohammed Alotibi*

**Paper 546t:** Catalysis of Calcium on  $\text{Fe}_2\text{O}_3/\text{Al}_2\text{O}_3$  Oxygen Carriers in Chemical Looping Combustion — *Zhifeng Zhang, Yifei Wang, Guangsu Yu, Fuchen Wang*

**Paper 546u:** Chemical Looping Partial Oxidation with Dry Reforming (CLPD) of Methane on a Ni-Promoted  $\text{Fe}_2\text{O}_3/\text{Al}_2\text{O}_3$  — *Jae W. Lee, Dohyung Kang, Hyun Suk Lim, Minbeom Lee*

**Paper 546v:** A Solid Mineral (limestone) As a Potential Catalyst for Biodiesel Production from Yellow Oleander Oil (*Thevetia peruviana*) — *Daniel Oyekunle*

**Paper 546w:** Effect of Reaction Time on the Yield of Biodiesel Produced from Yellow Oleander Seed Oil. — *Daniel Oyekunle*

**Paper 546x:** Liquid Lipase-Catalyzed Esterification of Oleic Acid with Methanol in the Presence of Superabsorbent Polymer for Biodiesel Production — *Chia-Hung Su, Dinh Thi My Huong, Hoang Chinh Nguyen*

**Paper 546y:**  $\text{CO}_2$  Utilization in a Chemical Looping System for Methane Conversion to High Purity Syngas Using an Iron Based Composite Metal Oxide — *Deven Baser, Zhuo Cheng, Liang-Shih Fan*

#### (547) Poster Session: Process Development

**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

Joe Schroer, Chair  
Shweta Karwa, Co-Chair

**Sponsored by:** Process Development Division

#### ■ ENERGY CONSUMING AND SUSTAINABLE SYSTEMS

**Paper 547a:** Catalytic Conversion of Glycerol to Value-Added Dicarboxylic Acids: Experimental Studies and Process Simulation on Energy Requirement and Environmental Impact — *Mengyuan Liu, Xin Jin, Chuanqin Ding, Bin Yin, Jingyao Wang, Chaohe Yang*

**Paper 547b:** Maintaining Operation Excellence in Badak LNG in Facing Leaner Gas Entrance — *Mohammad Arief Setiawan, Danu Purwanugraha, Rendra Prasetyo*

**Paper 547c:** Evaluation of  $\text{CO}_2$  Capture and Storage Systems for Existing Thermoelectric Plants in Mexico — *Adriana Palacios-Rosas, Nelly Ramirez-Corona, Pablo Emmanuel Álvarez-Alonso*

**Paper 547d:** Application of Ion Selective Electrodes (ISEs) for Real Time Monitoring of Flue Gas Desulfurization (FGD) Wastewater — *Shanta Mazumder, M. Toufiq Reza*

**Paper 547e:** Energy Efficiency Calculation of a Combined Heat and Power(CHP) Plant Integrated with Torrefaction Process Using Aspen PLUS — *Dong Yuel Yun, Quang-Vu Bach, Chul-Jin Lee*

**Paper 547f:** Utility System Optimization Under Air Quality Considerations — *Mona Naser, Konstantinos E. Kakosimos, Patrick Linke*

#### ■ REACTION AND SEPARATIONS DEVELOPMENT

**Paper 547g:** Design of Extractive Distillation Processes Using Simulated Annealing and a Rigorous Process Simulator — *Xiao-Ling Yang, Jeffrey D. Ward*

**Paper 547h:** Comparison of Batch Vs Continuous Operation for the Acquisition of Robust Reaction Kinetics in the Production of Succinimide Dispersants — *Zibo Zhen, Edmund Sam-Gyandoh, Sam Batchelder, Nasser Al-Azri, Hari C. Mantri Pragasada, Robert M. Enick, Cliff Kowall, Götz Vesper*

**Paper 547k:** Implementation of a Control Strategy for a Multitasking Reactive Distillation Column with an Intermediate Condenser — *Miguel E. Ortega-González, Nelly Ramírez-Corona, Adriana Palacios-Rosas, Juan Gabriel Segovia-Hernández*

**Paper 547l:** Aqueous Benzyl Alcohol Oxidation Using Polymer Nanoreactors: Towards Multifunctional Nanoscale Reactors — *Andrew Harrison, Matthew Nguyen, Tien Vuong, Christina Tang*

#### (548) Poster Session: Sustainability and Sustainable Biorefineries

**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, Exhibit Hall B

Ashley M. Pennington, Chair  
Simona Liguori, Co-Chair  
Nastassja Lewinski, Co-Chair

**Sponsored by:** General

#### ■ BIOFUELS AND BIOPRODUCTS

**Paper 548a:** Integration of  $\text{CO}_2$  Biomass Gasification with SOFC as a Viable Pathway for Carbon Capture and Sequestration — *Monica Abdallah, Amanda Simson*

**Paper 548b:** Energetic and Environmental Assessment of Biomass to Ethanol Processing in the Sugar-Cane Industry — *Jaykumar Mavani, Jorge E. Gatica, Michel Kahwaji Janho, Mauricio Colombo, Fernando Daniel Mele, María Rosa Hernández*

**Paper 548c:** Effects of Overliming and Activated Carbon on Carbonyl Inhibitors Removal and Butanol Fermentation in Biomass Hydrolysates — *Yu Zhang, Maobing Tu*

**Paper 548d:** Sustainable Evaluation of Environmental and Occupational Risks Scheduling Flexible Job SHOP Manufacturing Systems — *German Coca, Omar D. Castrillon, Santiago Ruiz, Josep M Mateo-Sanz, Laureano Jiménez, Carlos Pozo Fernández*

**Paper 548e:** Green and Sustainable Nanomaterials — *Nastassja Lewinski, Cory Jensen*

**Paper 548f:** Methods for Tracking the Evolution of Refractory REE Mineral Decomposition in Strong Acid Media — *Joanne Gamage McEvoy, Yves Thibault*

**Paper 548g:** Optimization of Dye Degradation Process By Oxidative Technology — *Mayur Yenkie*

**Paper 303a:** Assessing the Effect of Substrate and Catalyst on Catalytic Waste Gasification — *Michael Matrona, Jorge E. Gatica, Mason Lang, Nilesch Valand*

**Paper 48e:** Site-Specific Cross-Linking and Immobilization of Agarase Enzymes for Conversion of *Gelidium Amansii* into Biologically-Active Sugars — *Rosemarie Ann I. Cuevas, Teklebrhan G. K. Weldemhret, Kris Niño G. Valdehuesa, Grace M. Nisola, Kristine Rose M. Ramos, Hiluf Tekle Fissaha, Won-Keun Lee, Wook-Jin Chung*

#### ■ VALORIZATION AND UTILIZATION OF WASTE

**Paper 548j:** Identifying and Addressing Potential Barriers Towards Commercialization of Novel, Thermocatalytic Non-Food Sugar to Acrylonitrile Process — *Jadid Samad, William Grieco, Amit Goyal*

**Paper 548k:** Electronic Waste to Nanoparticles: Influence of Precursor Purity on Nanoparticle Synthesis — *Kathryn Dill, Nastassja Lewinski*

**Paper 548l:** Techno-Economic Analysis of Biofuels Production Via Localized Fast Pyrolysis and Electrocatalytic Upgrading — *Sabyasachi Das, Christopher M. Saffron*

**Paper 548m:** The Valorization of Sprayed Lignins with Ozone — *Julian Silverman, Bala Subramaniam*

**Paper 548n:** DES Pretreatment Leading to Highly Concentrated Sugar Hydrolysate and Valorizable Lignin — *Caixia Wan, Zhu Chen, Xianglan Bai, A Lusi*

**Paper 548o:** Towards Lignin Valorization: Pyrolytic Depolymerization and Electrochemical Upgrading of Lignins Extracted from Pretreated Biomass to Valuable Intermediates — *Mahlet Garedew, James E. Jackson, Christopher M. Saffron*

**Paper 548p:** Supply Chain Analysis and Process Evaluation for Advancing Sustainable Material Recovery from Post-Consumer Waste — *Gerardo J. Ruiz-Mercado, Apoorva Sampat, Victor M. Zavala*

**Paper 548z:** Optimization Based Improved Water Recycle Strategies for Modern Oil Refineries — *Abhilasha Maheshwari, Vijaysai Prasad, Ravindra D. Gudi*



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.



## ■ SUSTAINABILITY METRICS AND PROCESS OPTIMIZATION

**Paper 548q:** Life Cycle Carbon Footprint of Renewable Electricity Generation from Aspen Forest Harvest in Wisconsin, USA — **Olumide Winjobi**, Michelle Cisz, Sigrid Resh, David R. Shonnard, Colin Phifer, Rodney Chimner

**Paper 548r:** A Life Cycle Cost Analysis of a Cattle-Based Anaerobic Digester Operation in Iowa — **Alvina Aui**, Mark Mba Wright

**Paper 548s:** Environmental Impact Assessment for High Conversion Synthesis of <10 Nm Silver Nanoparticles Using Microwave Assisted Heating By Life Cycle Techniques — **Adarsh Bafana**, Shishir V Kumar, Prasad P Pawar, Sila Temizel-Sekeryan, Si A. Dahoumane, Liv Haselbach, Clayton S Jeffries

**Paper 548t:** Anhydrous Bio-Ethanol Production: Life Cycle Analysis of Distillation and Dehydration Steps — **Jaykumar Mavani**, Jorge E. Gatica, Michel Kahwaji Janho, Mauricio Colombo, Fernando Daniel Mele, María Rosa Hernández

**Paper 548u:** Planning, Design and Operation of Sustainable and Efficient Multi-Product Rice Value Chains Using Multi-Objective Spatio-Temporal Optimisation — **Stephen S. Doliente**, Sheila Samsatli

**Paper 548v:** Kinetic Parameter Estimation for Electrocatalytic Hydrogenation of Model Compounds Derived from Fast Pyrolysis of Biomass — **Sabyasachi Das**, Christopher M. Saffron

**Paper 548w:** The Search for Sustainability in an Integrated Economic-Ecologic-Social Model through the Use of Feedback Loops — **Pablo T Rodriguez-Gonzalez**, Vicente Rico-Ramirez, Ramiro Rico-Martinez, Urmila M. Diwekar

**Paper 548y:** Water Pinch Points in Thermoelectric Power Generation — **Jocelyn Kate Mackay**, Briggs White, Dale Keairns, Katrina Krulla, Massood Ramezan

**Paper 204a:** Process Design Optimization for *Saccharina japonica* Based Biorefinery: A Superstructure Based Approach — **Rofice Dickson**, J. Jay Liu

**Paper 394c:** Optimization of Macroalgae Based Biorefinery Producing Fuel and Chemicals with Zero Carbon Emissions Potential — **Rofice Dickson**, J. Jay Liu

**(549) Ammonia Energy Global Demonstrations**  
Wednesday, Oct 31, 3:30 PM  
David L. Lawrence Convention Center, 318

Trevor Brown, Chair

**Sponsored by:** NH3 Energy+

**3:30 Paper 549a:** Test Results of the Ammonia Mixed Combustion at Mizushima Power Station Unit No.2 and Related Patent Applications — **Hiroaki Tanigawa**

**3:45 Paper 549b:** Performance of Ammonia - Natural Gas Co-Fired Gas Turbine for Power Generation — **Shintaro Ito**, Masahiro Uchida, Shogo Onishi, Soichiro Kato, Toshio Fujimori, Hideaki Kobayashi

**4:00 Paper 549c:** Rapid Ramp NH<sub>3</sub> Prototype Reactor Update — **Joseph Beach**, Jonathan Kintner, Adam Welch

**4:15 Paper 434d:** Realisation of Large-Scale Green Ammonia Plants — **Markus Will**

**4:30 Paper 549d:** Demonstration of CO<sub>2</sub>-Free Ammonia Synthesis Using Renewable Energy-Generated Hydrogen — **Mototaka Kai**, Yasushi Fujimura, Takayoshi Fujimoto, Hideyuki Takagi, Tetsuya Nanba, Yuichi Manaka

**4:45 Paper 549f:** Design Optimization of an Ammonia-Based Distributed Sustainable Agricultural Energy System — **Matthew J. Palys**, Anatoliy Kuznetsov, Joel Tallaksen, Michael Reese, Prodromos Daoutidis

**5:00 Paper 549g:** Evaluation of the Cement Clinker Fired in the Combustion Furnace of Heavy-Oil and NH<sub>3</sub> — **Hiroki Kujiraoka**, Tatsuro Izumi, Yuya Yoshizuru, Takeshi Suemasu, Makoto Ueda, Toyooki Niki, Takayasu Itou, Masayuki Nishio, Ryuichi Murai, Fumiteru Akamatsu

**5:15 Paper 549h:** Ammonia-to-Hydrogen System for Fcev Refuelling — **Michael D. Dolan**

**(550) Adsorbent Materials for Sustainable Energy and Chemicals**  
Wednesday, Oct 31, 3:30 PM  
David L. Lawrence Convention Center, 301

F. Handan Tezel, Chair  
Youssef Belmabkhout, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**3:30 Paper 550a:** Investigating the Effect of Cu and Ce Loading in Mesoporous Y Zeolite for the Adsorptive Desulfurization of 4,6-Dimethyldibenzothiohene — **Kevin X. Lee**, George Tsilomelekis, Julia A. Valla

**3:45 Paper 550b:** Role of Amine Structure on Hydrogen Sulfide Capture from Dilute Gas Streams Using Solid Adsorbents — **Claudia Okonkwo**, Christopher W. Jones, Guanghui Zhu, Chukwuemeka Okolie, Achintya Sujan

**4:00 Paper 550c:** Hydrogen Sulfide Removal from Biogas on "Molecular Basket" Sorbents — **Wenying Quan**, Xiaoxing Wang, Chunshan Song

**4:15 Paper 550d:** Preparation and Characterization of Novel Clinoptilolites: Treatment of Natural Gas Type Mixtures Using Inorganic Membranes — **Dean Kennedy**, Maja Mujcin, Talal Omar, Christa Abou Zeid, F. Handan Tezel

**4:30 Paper 550e:** Copper Modified Activated Carbon for Hydrogen Purification — **Frederico Relvas**, Carlos M. Silva, Roger D. Whitley, Adélio Mendes

**4:45 Paper 550f:** Zeolite X Molecular Sieves As Active Materials in the Separation of Effluent Gases from the OCM Process — **Hector D. Diaz Ortiz**, Karla D. Guerrero G., Cristian C. Rodriguez, Hamid Godini, Erik Esche, Gerardo Rodriguez, Jens-Uwe Repke, Alvaro Orjuela, Oliver Görke, Jose H. Ramirez F.

**5:00 Paper 550g:** Carbon Dioxide Adsorption at Elevated Temperatures for Vehicle Exhaust Gas Treatment — **Christina Reynolds**, Nathaniel Sunderlin, Christian Lastoskie

**5:15 Paper 550h:** Adsorption of Rare Earth Elements in Phosphorous Functionalized Nanoporous Carbon — **Dipendu Saha**, Sel Didem Akkoyunlu

**(551) Advanced Inorganic Materials for Membrane Gas Separation**  
Wednesday, Oct 31, 3:30 PM  
David L. Lawrence Convention Center, 303

Ali Rownagi, Co-Chair  
Xueyi Zhang, Co-Chair  
Seok-Jhin Kim, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 551a:** Large-Area Single Layer Graphene Membrane By Crack-Free Transfer for Gas Mixture Separation — **Shiqi Huang**, Kumar Varoon Agrawal

**3:44 Paper 551b:** Rapid Synthesis of Mixed Linker Zeolitic-Imidazolate Frameworks (ZIFs) Membranes with Tunable Gas Separations — **Febrian Hillman**, Jordan Brito, Hae-Kwon Jeong

**3:58 Paper 551c:** Suppression and Reversal of Physical Aging in Carbon Molecular Sieve Hollow Fiber Membranes — **Samuel Hays**, Oishi Sanyal, Chen Zhang, Graham Wenz, Nicholas Doss, Nicholas Leon, William J. Koros

**4:12 Paper 551d:** Vapor Phase Processing of Zeolitic Imidazolate Framework Membranes — **Xiaoli Ma**, Prashant Kumar, Nitish Mittal, Alexandra Khlyustova, Prodromos Daoutidis, K. Andre Mkhoyan, Michael Tsapatsis

**4:26 Paper 551e:** ALPO-18 Membrane for Gas Separations — **Masahiko Matsukata**, Kei Toshihara, Motomu Sakai

**4:40 Paper 551f:** Two-Stage Varying-Temperature Synthesis of High-Performance SAPO-34 Membranes for H<sub>2</sub>/N<sub>2</sub> Separation at High Temperature — **Ji Jiang**, Syed Islam, Qiaobei Dong, Shiguang Li, Naomi Klinghoffer, Xinhua Liang, Miao Yu

**4:54 Paper 551g:** Molecular Layer Deposition Modified SAPO-34 Membranes on Ceramic Hollow Fibers for Separation of H<sub>2</sub>/N<sub>2</sub> Mixtures at High Temperature and High Pressure — **Syed Z. Islam**, Ji Jiang, Qiaobei Dong, Huazheng Li, Shiguang Li, Naomi Klinghoffer, Xinhua Liang, Miao Yu

**5:08 Paper 551h:** Enhanced Gas Separation Performance of Mixed-Linker Zeolitic Imidazolate Framework ZIF Membranes Via Post Synthetic Ligand Exchange — **Moon Joo Lee**, Yu-Chen Hsu, Mohamad Rezi Abdul Hamid, Stephanie Bates, Hae-Kwon Jeong

**5:22 Paper 551i:** Relevance of “Cross-over” Pores in CMS Membrane Transport Properties — **Oishi Sanyal**, Samuel Hays, Graham Wenz, William J. Koros

**5:36 Paper 551j:** Mixed Matrix Membranes Formed from Branched HKUST-1 for Improved Plasticization Resistance and Transport Performance — **Won Seok Chi**, Benjamin J. Sundell, Ke Zhang, Daniel J. Harrigan, Steven C. Hayden, Zachary Smith

**(552) Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications**

**Wednesday, Oct 31, 3:30 PM**

Omni William Penn Hotel, Conference Center B

Yakov Lapitsky, Chair  
Sepideh Razavi, Co-Chair  
Jaime Juárez, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 552a:** Chloride and Hexadecylamine Promote the Solution-Phase Growth of Copper Nanowires — **Zihao Chen**, Myung Jun, Benjamin Wiley, Kristen Fichthorn

**3:45 Paper 552b:** Role of Long-Chain Alkylamines in the Growth of Fivefold-Twinned Cu Nanowires — **Tianyu Yan**, Kristen Fichthorn

**4:00 Paper 552c:** Structures and Dynamics of Boehmite Crystal Aggregation — **Jaehun Chun**, Elias Nakouzi, Jennifer Soltis, Benjamin Legg, Gregory K. Schenter, Xin Zhang, Trent R. Graham, Kevin Rosso, Lawrence Anovitz, James J. De Yoreo

**4:15 Paper 552d:** Topological Transitions in Densely Packed Anisotropic Colloids — **William Zygmunt**, Erin G. Teich, Greg van Anders, Sharon C. Glotzer

**4:30 Paper 552e:** Reconfigurable Light Diffraction Response of Ellipsoidal Colloids By Electric Field Assisted Assembly — **Peng-Kai Kao**, Bryan Vansaders, Michael Durkin, Sharon C. Glotzer, Michael J. Solomon

**4:45 Paper 552f:** Influence of Cap Weight on the Motion of a Janus Particle Very Near a Wall — **Aidin Rashidi**, Sepideh Razavi, Christopher L. Wirth

**5:00 Paper 552g:** Investigation on the Synergistic Effect of Surfactant and Amphiphilic Nanoparticles at Oil-Water Interface By Dissipative Particle Dynamics Simulations — **Tuan V. Vu**, Dimitrios V. Papavassiliou

**5:15 Paper 552h:** Effect of Amphiphilicity and Janus Cap Orientation on Janus Particles at an Air-Water Interface — **Ellen M. Knapp**, Raymond R. Dagastine, Ilona Kretzschmar, Raymond Tu

**5:30 Paper 552i:** Studying the Orientation of a Janus Particle Near a Wall Under Varying Flow Conditions — **Zohreh Jalilvand**, Joel Koplik, Ilona Kretzschmar

**5:45 Paper 552j:** The Hindered Translational and Rotational Dynamics of Nano-Rods Diffusing Near a Solid-Liquid Interface in Aqueous Solution — **Christopher Bolton**, **Raymond R. Dagastine**

**(553) Biomanufacturing**

**Wednesday, Oct 31, 3:30 PM**

Westin Convention Center, Pennsylvania East

Nitin Agrawal, Chair

**Sponsored by:** Immunotherapy

**3:30 Paper 553a:** Challenges in Continuous Manufacturing of Biologics: Summary of NASEM Workshop — **G. V. Rex Reklaitis**

**4:00 Paper 553b:** Ruben Carbonell: Invited Talk on Immunotherapy Biomanufacturing — **Ruben G. Carbonell**

**4:30 Paper 553c:** Leveraging Biomaterial Stability and Retention in Lymph Nodes to Control Immunity — **Christopher Jewell**

**5:00 Paper 553d:** Improving Homogeneous Differentiation of Stem Cells By CRISPR-Mediated Knockout — **Christina Chan**, Ryan Thompson

**5:30 Paper 553e:** Liposome Targeted Proliferation of Cytotoxic T Cells — **Nitin Agrawal**

**(554) Biomaterial Scaffolds for Tissue Engineering II: Bioactive and Drug-Eluting Materials**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 328

Ryan Koppes, Co-Chair  
Jungwoo Lee, Co-Chair  
Tadas Kasputis, Co-Chair

**Sponsored by:** Biomaterials

**3:30 Paper 554a:** Design of a Two-Phase System for the Sustained Delivery of Growth Factors for Bone Tissue Engineering Applications — **Tinke-Marie De Witte**, **Angela Wagner**, Camila Parra, Lidy E. Fratila-Apachitei, Amir A. Zadpoor, Nicholas A. Peppas

**3:48 Paper 554b:** Fabrication of PNIPAM Electrospun Nanofiber Substrates for Temperature-Mediated Cell Release — **Rachel Young**, **Lauren Anderson**

**4:06 Paper 554c:** Engineering Microenvironments to Regulate Mesenchymal Stem Cell Secretome — **Malak Nasser**, Gargi Ghosh

**4:24 Paper 554d:** Tissue-Engineered Perfusable Small Diameter Blood Vessels for Vascular Applications — **Ebrahim Mostafavi**, Nasim Annabi

**4:42 Paper 554e:** Application of Hydrogen Sulfide Releasing Materials in Complex Bone Regeneration — **Soheila Aliakbarighavimi**, Ethan Lungren, Trent Faulkner, Brittany Allen, Jessica Stromsdorfer, Ram Rao Tata, Bret Utery

**5:00 Paper 554f:** Magnetically Responsive Gels for Enhancing Osteo-Differentiation By Controlling the Timing of Recruitment and Differentiation Factor Deliveries — **Seyedeh Zahra Moafi Madani**, Anne Reisch, Stephen Kennedy

**5:18 Paper 554g:** Integrated Effects of Matrix Mechanics and Sustained Release of Bioactive Factors on Accelerating Wound Healing — **Victoria Sears**, Gargi Ghosh

**5:36 Paper 554h:** Bioactive Two-Dimensional (2D) Nanoparticles to Modulate Differentiation of Human Mesenchymal Stem Cells — **Akhilesh K. Gaharwar**

**(555) Bionanotechnology for Gene and Drug Delivery II**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 309

Elizabeth Nance, Chair  
Joo-Youp Lee, Co-Chair

**Sponsored by:** Bionanotechnology

**3:30 Paper 555a:** Optimization of Liposome-Hollow Gold Nanoparticle for mRNA Delivery — **Anisha Veeren**, Mark Osborn, Sarah Merkel, JeongEun Shin, Joesph A. Zasadzinski

**3:45 Paper 555b:** Lipid Nanoparticle Ionization at Endosomal pH Is a Cell-Free Predictor of mRNA Delivery Efficacy In Vivo — **Khalid A. Hajj**, Rebecca Ball, Sarah Deluty, Shridhar Singh, Christopher Knapp, Kathryn A. Whitehead

**4:00 Paper 555c:** pH Responsive Polycationic Nanoparticles for siRNA Delivery in Inflammatory Bowel Diseases — **Aaliyah B. Shodeinde**, Angela Wagner, Nicholas A. Peppas

**4:15 Paper 555d:** Lipid Nanoparticle Mediated Drug Delivery for Targeting Inflammation Site in Atherosclerosis — **Rashi Porwal**, Stephen L. Hayward, Xiang-der Liu, Yiannis Chatzizisis, Srivatsan Kidambi

**4:30 Paper 555e:** Internalization and Endocytic Trafficking of 3WJ RNA Nanoparticles for siRNA Delivery — **Landon A. Mott**, Peixuan Guo, Daniel W. Pack

**4:45 Paper 555f:** Synthesis of Poly(Aspartic Acid)-Doxorubicin Prodrug for Sequential Delivery of Afatinib and Doxorubicin — **Mina Jafari**, Vishnu Sriram, Joo-Youp Lee

**5:00 Paper 555g:** Co-Delivery of 2-DG and V9302 Via a Prodrug Micellar Formulation for Synergistic Targeting of Metabolism in Cancers — **Zhangyi Luo**, Yang Wu-yue Liu, Yan He, Jingjing Sun, Song Li

**5:15 Paper 555h:** Engineering PEO-Pdlla Nanoparticles Containing the PI3K Inhibitor LY294002 — **Austin Fergusson**, Ami Jo, Richey M. Davis

**5:30 Paper 555i:** Targeting Tumor Associated Macrophages with PAMAM Dendrimers Improves Therapeutic Efficacy in Glioblastoma — **Kevin Liaw**, Rishi Sharma, Rajsekhar Reddy, Sujatha Kannan, Rangaramanujam Kannan

**5:45 Paper 555j:** Programming Tumor-Clearing Macrophages with Targeted Gene Therapy — **Fan Zhang**, Michael Coon, Sirkka Stephan, Smitha Pillai, Matthias Stephan

**(556) Cells, Organs, and Labs on a Chip II: Tissues and Diseases**

**Wednesday, Oct 31, 3:30 PM**

Westin Convention Center, Somerset

Heather Fahlenkamp, Co-Chair  
Grissel Trujillo-de Santiago, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**3:30 Paper 556a:** Neuron-on-a-Chip: A Novel Microfluidic Device for Neural 3D Tissue Culture — **David Choy**, Buentello, Matias José Lobo-Zegers, Mariana García-Corral Islas, Andrea Jiménez Fernández, Mario Moisés Alvarez, Grissel Trujillo-de Santiago

**3:48 Paper 556b:** Microphysiological Systems for Emulating Human Tissues and Diseases — **Yu Shrike Zhang**

**4:06 Paper 556c:** Towards Interactive Tissue Patterning Via Spatially Defined Addressable Microfluidic Delivery of Chemical Signals — **Nhat-Anh N. Tong**, Long Quang Pham, Vatsal Shah, Paul Abatemarco, Roman Voronov

**4:24 Paper 556d:** Towards Rapid Prototyping of a Patient Derived Gut-on-a-Chip — **Sanjin Hoscic, Marissa Puzan, Fanny Zhou, David Breault, Shashi Murthy, Abigail Koppes**

**4:42 Paper 556e:** Tunable Attachment of Living Cells to Electroactive Surfaces — **Ariel Furst, Matthew Francis**

**5:00 Paper 556f:** Human Breathing Lung-on-a Chip for Inhalation Drug Delivery — **Chun-Kai Lin, Bing-Syuan Ni, Hsin-Lin Hsieh, Jen-Huang Huang**

**5:18 Paper 556g:** High-Throughput Toxicity Testing of Chemicals and Mixtures in Organotypic Multi-Cellular Cultures of Primary Human Hepatic Cells — **Sophia Orbach, Marion Ehrich, Padmavathy Rajagopalan**

**5:36 Paper 556h:** Multiscale Image-Based Simulation of Transient PDGF-BB Gradient Formation Explains How Fibroblasts Affect Each Other in Making Directional Decision during Chemotaxis — **Long Quang Pham, Lydia N. Rodrigues, Vishnu Deep Chandran, David Chege, Nhat-Anh N. Tong, Roman Voronov**

#### (557) Continuous Processing Technologies Applied in Drug Product Development II

**Wednesday, Oct 31, 3:30 PM**  
Westin Convention Center, Washington

Sarang Oka, Chair  
Carla Luciani, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 557a:** Continuous Mixing Technology: Process Design with Discrete Element Method (DEM) Simulations — **Peter Toson, Eva Siegmann, Martina Trogrlic, Dalibor Jajcevic, Johannes G. Khinast, Pankaj Doshi, Daniel O. Blackwood, Mary T. am Ende**

**3:51 Paper 557b:** Continuous Mixing Technology: Residence Time Distribution Modeling — **Peter Toson, Eva Siegmann, Martina Trogrlic, Dalibor Jajcevic, Johannes G. Khinast, Pankaj Doshi, Daniel O. Blackwood, Alex Bonnassieux, Mary T. am Ende**

**4:12 Paper 557c:** Residence Time Distribution Determination in Pneumatic Conveying Processes for the Continuous Manufacturing of Pharmaceutical Products — **Eric Jayjock, Jack Qian, Nicholas Pick, Brian Sauerborn, Keirnan LaMarche**

**4:33 Paper 557d:** RTD Based Control System for Continuous Pharmaceutical Manufacturing Process — **Ravendra Singh, Fernando J. Muzzio**

**4:54 Paper 557e:** Developing a System Based Model for Continuous Direct Compression – Going Beyond Tablet Assay — **Gavin K. Reynolds**

**5:15 Paper 557f:** Twin-Screw Continuous Granulations: Technological and PAT Developments — **Balázs Démuth, Brigitta Nagy, Lajos Madarász, Réka Á. Fazekas, Márk Kovács, András Domokos, Attila Farkas, György Marosi, Hajnalka Pataki, Zsombor K. Nagy**

**5:36 Paper 557g:** The Continuous Manufacturing of Pharmaceutical Capsules — **Eric Jayjock, Nicholas Pick, Jack Qian, Zhonghui Huang, Keirnan LaMarche**

#### (558) Developing Process Control Strategies for Drug Substance Manufacture

**Wednesday, Oct 31, 3:30 PM**  
Westin Convention Center, Fayetteville

Kevin Seibert, Chair  
Huiquan Wu, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 558a:** Design and Implementation of a Control Strategy Using Risk-Based Probabilistic Design Principles: A Case Study in the Manufacturing an API with a Critical Impurity — **Federico Lora Gonzalez, Jose E. Tabora, Eric C. Huang, Steven R. Wisniewski, Thomas M. Razler, Brendan C. Mack**

**3:51 Paper 558b:** Proteomics Guided Process Engineering for Anti-HER2 Antibody Production — **Jianfa Ou, Ningning Xu, Yingnan Si, Kahyong Goh, Patrick Ernst, Lufang Zhou, X. Margaret Liu**

**4:12 Paper 558c:** Formation Mechanism and Phase Transformation Behaviors of Polymorphs of Esomeprazole Sodium — **Qi Liu, Shuyi Zong, Hao Wu, Jingkan Wang, Hongxun Hao**

**4:33 Paper 558d:** Process Modeling of a Continuous Drug Substance Manufacturing Process — **Nima Yazdanpanah, Thomas O'Connor, Celia N. Cruz**

**4:54 Paper 558e:** Green Process Development and Characterization of an Alkylation Reaction to Improve API Impurity Control — **Cuixian Yang, Michael Ward, Guy Humprey, Bharath Krishnamurthi, Erik Dienemann, Timothy Wright, Nicholas Rogus, Anne Mohan, Peter Malignes**

**5:15 Paper 558f:** Leveraging PAT for Efficient Process Development Workflows — **James C. Marek, Eric G. Moschetta, Travis B. Dunn**

**5:36 Paper 558g:** On-Line FTIR for Accurate Fundamental Kinetic Analysis, Real-Time Process Monitoring, and Process Controls Justification in Pharmaceutical Manufacturing — **Eric G. Moschetta, James C. Marek, Travis B. Dunn**

#### (559) Drug Delivery III: Systems for Administration

**Wednesday, Oct 31, 3:30 PM**  
Westin Convention Center, Cambria

Forrest Kievit, Co-Chair  
Sidi Bencherif, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**3:30 Paper 559a:** Nanoengineered Biomaterials for Sustained and Prolong Therapeutic Delivery — **Akhilesh K. Gaharwar**

**3:48 Paper 559b:** Microneedles for Allergen Immunotherapy: In Vivo Efficacy in Mouse Models of Airway Allergy — **Akhilesh Shakya, Chang Hyun Lee, Harvinder Singh Gill**

**4:06 Paper 559c:** Strawberry Polyphenols As Intestinal Permeation Enhancers for Oral Drug Delivery — **Nicholas G. Lamson, Rebecca Ball, Kanika Suri, Anna Zhang, Vishal Ahuja, Adrian Berger, Kathryn A. Whitehead**

**4:24 Paper 559d:** Design, Structure, Material Strength of Dissolvable Microneedle Patch Vaccine Delivery Systems: From Fabrication to Characterization of Microscale Transdermal Patches — **Mohammad Mofidfar, Mark R. Prausnitz**

**4:42 Paper 559e:** Highly Targeted Ocular Drug Delivery By Iontophoresis and Swollen Hydrogel Pushing in the Suprachoroidal Space — **Jae Hwan Jung, J. Jeremy Chae, Mark R. Prausnitz**

**5:00 Paper 559f:** Modulation of Neural Activity Via on-Demand Magnetothermal Drug Release — **Gabriela Romero-Urbe**

**5:18 Paper 559g:** Filament Extension Atomizer: Novel Aerosol Generation from Viscous Fluids and Applications in Biotechnology — **Jerome Unidad, Ravi Neelakantan, Jamie Kalb, Michael Benedict, David Johnson**

**5:36 Paper 559h:** Photodynamic Therapy and Drug Delivery Via Multifunctional Optical Fibers for Cancer Treatment — **Ai Lin Chin, Rong Tong**

#### (560) Dynamics, Reduction, and Control of Distributed Parameter Systems

**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, 408

Panagiotis D. Christofides, Chair  
Stevan Dubljevic, Co-Chair  
Wei Dai, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

**3:30 Paper 560a:** Graph Representation and Decomposition of Diffusion-Convection-Reaction Processes for Distributed Control — **Manjiri Moharir, Davood Babaei Pourkargar, Ali Almansoori, Prodromos Daoutidis**

**3:48 Paper 560b:** Machine Learning-Based Model Predictive Control of Distributed Chemical Processes — **Anh Tran, Yangyao Ding, Panagiotis D. Christofides**

**4:06 Paper 560c:** Optimization-Based Sensor/Actuator Scheduling and Control of Sampled-Data Distributed Processes — **Da Xue, Nael H. El-Farrah**

**4:24 Paper 560d:** Adaptive Model Reduction for Dissipative PDE Systems with Strong Convective Phenomena — **Manda Yang, Antonios Armaou**

**4:42 Paper 560e:** Equation-Free Multiparametric Model Predictive Control for Dissipative PDEs — **Panagiotis Petsagkourakis, Constantinos Theodoropoulos**

**5:00 Paper 560f:** Product Uniformity in PECVD Systems: Applying Run-to-Run Control to a Multiscale Three-Dimensional CFD Model — **Marquis Crose, Anh Tran, Yangyao Ding, Panagiotis D. Christofides, Weiqi Zhang**

**5:18 Paper 560g:** Process Monitoring and Leakage Diagnosis for Distributed Pipeline System Based on Discrete Observer and Moving Horizon Estimation — **Junyao Xie, Stevan Dubljevic**

**5:36 Paper 560h:** Dynamic Modeling and Control of a Natural Gas Combined Cycle (NGCC) Power Plant with a Damage Model — **Yifan Wang, Debansu Bhattacharyya, Richard Turton**



**(561) Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions II**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 306

Gang Wu, Chair  
Hong Yang, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

**3:30 Paper 561a:** Towards Establishing Apparent Hydrogen Binding Energy As the Descriptor for Hydrogen Oxidation/Evolution Reactions (*Invited*) — **Jie Zheng, Jared Nash, Bingjun Xu, Yushan Yan**

**3:50 Paper 561b:** Enhancing Complete Oxidation of Ethanol during the Electrochemical Reforming Process for Hydrogen Production (*Invited*) — **Xiaowei Teng**

**4:10 Paper 561c:** Mechanistic Studies of Fe Based LDH and Phosphosulfides for Oer and HER Using *in Situ operando* synchrotron X-Ray Spectroscopy and Scattering (*Invited*) — **Zhenxing Feng**

**4:30 Paper 561d:** Effect of Hydrogen Diffusion on Hydrogen Oxidation/Evolution Kinetics (*Invited*) — **Jie Zheng, Jared Nash, Junhua Wang, Xuan Yang, Yushan Yan, Bingjun Xu**

**4:50 Paper 561e:** Combining Experiment and Simulations to Determine the Role of Adsorbed Hydroxide in Alkaline Hydrogen Electrocatalysis (*Invited*) — **Maureen H. Tang, Joshua Snyder, Saad Intikhab, Luis Rebolgar**

**5:10 Paper 561f:** Quantifying Confidence in Density Functional Theory Predicted Surface Pourbaix Diagrams at Solid-Liquid Interfaces: Implications for Electrochemical Processes — **Olga Vinogradova**

**5:30 Paper 561g:** Mechanistic Study of Non-Precious Transition Metal/Nitrogen Doped Carbon Electrocatalysts for Oxygen Reduction Reaction (*Invited*) — **Guofeng Wang**

**5:50 Paper 561h:** Multiscale Principles to Boost Reactivity in Gas-Involving Energy Electrocatalysis (*Invited*) — **Cheng Tang, Haofan Wang, Qiang Zhang**

**(562) Electronic and Photonic Materials Devices and Theory**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 330

Andrej Lenert, Chair  
Sang Eon Han, Co-Chair  
James Dorman, Co-Chair

**Sponsored by:** Electronics and Photonics

**3:30 Paper 562a:** *Invited:* Effective Radiative Cooling By Paint-Format Microsphere-Based Photonic Random Media — **Sang Eon Han, Sarun Atiganyanun, John Plumley, Seok Jun Han, Kevin Hsu, Jacob Cytrynbaum, Thomas Peng, Sang M Han**

**3:50 Paper 562b:** Highly Stretchable, Sensitive, and Self-Healable Wearable Strain Sensor Based on an Elastomeric Hierarchical Conductive Nanofiber Network — **Yang Lu, Seungwoon "Paul" You, Steven Diklich, Ju-Won Jeon, Evan K. Wujcik**

**4:10 Paper 562c:** Unraveling Excitation Energy Transfer Mechanisms in Plasmonic Nanoantennas — **Niranjan V. Ilawe, Bryan M. Wong, M. Belen Oviedo**

**4:30 Paper 562d:** Pulse Dynamics of Electric Double Layer on Graphene FETs — **Ke Xu, Md Mahbul Islam, David Guzman, Alan Seabaugh, Alejandro Strachan, Susan Fullerton-Shirey**

**4:48 Paper 562e:** Nanoantennae-Induced Hot Carriers and Nonlinear Susceptibility in 2D Materials — **D. Keith Roper, Gregory T. Forcherio, Jeremy Dunklin, Yannick Mugnier, Ronan Le Dantec, Luigi Bonacina**

**5:06 Paper 562f:** Electric Double Layer Gating of Transition Metal Dichalcogenide Field-Effect Transistors Using a Monolayer Solid-State Electrolyte — **Jierui Liang, Ke Xu, Susan Fullerton-Shirey**

**5:24 Break**

**5:42 Paper 562h:** Fabrication and Characterization of Ionomer-Gated MoTe<sub>2</sub> Field Effect Transistors — **M. Eli Bostian, Ke Xu, Hangjun Ding, James R. McKone, Eric J. Beckman, Susan Fullerton-Shirey**

**(563) Emerging Tools and Enabling Technologies in Synthetic Biology: Design of Complex Circuits**

**Wednesday, Oct 31, 3:30 PM**

Westin Convention Center, Westmoreland West-Central

Thomas J. Mansell, Chair  
Nicholas R. Sandoval, Co-Chair

**Sponsored by:** Bioengineering

**3:30 Paper 563a:** Investigation of Unique Interspecies Interactions in a Synthetic and Syntrophic *Clostridium* Co-Culture — **Kamil Charubin, Eleftherios Terry Papoutsakis**

**3:48 Paper 563b:** Application and Validation of a Genome-Wide CRISPR-Cas9 Library for the Oleaginous Yeast *Yarrowia Lipolytica* — **Cory Schwartz, Ian Wheeldon**

**4:06 Paper 563c:** Highly Multiplexed CRISPR-Cas9 Applications with Extra Long Sgrna Arrays — **Alexander Reis, Sean Halper, Grace Vezeau, Daniel Cetnar, Ayaan Hossain, Phillip Clauer, Howard Salis**

**4:24 Paper 563d:** Synthetic Biology Framework for Engineering Post-Translational Circuits — **Nichole Daringer, Caleb J. Bashor, James Collins**

**4:42 Paper 563e:** Computational Modeling of Synthetic Gene Circuits to Improve Stem Cell Differentiation — **Mihe Hong, Joseph J. Muldoon, Joshua N. Leonard**

**5:00 Paper 563f:** An *in vitro* Transcriptional Regulatory Network for Modular Control of Synthetic Signals — **Samuel Schaffter, Rebecca Schulman**

**5:18 Paper 563g:** Design Platforms for Modular Cell Engineering and Precise CRISPR Genome Editing of Single and Consortia of Organisms — **Cong T. Trinh**

**(564) Energetic Materials: Engineered Particles and Interfaces I**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 412

Edward Dreizin, Chair  
Lori J. Groven, Co-Chair

**Sponsored by:** Energetics

**3:30** Introductory Remarks

**3:35 Paper 564a:** The Synthesis and Properties of Cyclic Nitramine Crystals with Metal Particles inclusions — **Alexander Vorozhtsov, Georgy Teplov**

**3:50 Break**

**4:05 Paper 564c:** Synthesis and Characterization of CL-20/Oxidant Crystals — **Clinton Chapman, Lori J. Groven**

**4:20 Break**

**4:35 Paper 564d:** Effect of Liquid Hydrocarbon-Based Process Control Agents on Characteristics of Mechanically Alloyed Al-Ti Powders — **Mehnaz Mursalat, Mirko Schoenitz, Edward Dreizin**

**4:50 Paper 564e:** Ignition and Combustion Mechanisms of Mg-Ca(IO<sub>3</sub>)<sub>2</sub> Reactive Nanocomposites — **Xinhang Liu, Mirko Schoenitz, Edward Dreizin**

**5:05 Paper 564f:** Graphene Oxide-Based Microwave Ignitable Energetic Materials with Thermally Switchable Ignition Characteristics — **Stuart J. Barkley, Keke Zhu, James B. Michael, Travis R. Sippel**

**5:20** Concluding Remarks

**(565) Free Forum on Engineering Education: Graduate Students**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 404

Laura Ford, Chair  
Adam St. Jean, Co-Chair  
Troy Vogel, Co-Chair

**Sponsored by:** Graduate Education

**3:30 Paper 565a:** Core Chemical Engineering Graduate Bridging Course: Development and Early Evaluation — **Hassan Golpour, Matthew Cooper, Lisa G. Bullard**

**3:55 Paper 565b:** Chemical Engineering Teaching Practicum Course: Reflections after Five Years — **Monica H. Lamm, Ashley Augspurger, Ian Schneider, Laura R. Jarboe**

**4:20 Paper 565c:** Teaching the Data Management Plan (DMP) to Graduate Students — **Joseph H. Holles, Lawrence Schmidt**

**4:45 Paper 565d:** Chemical Accounting with an Open-Access Life Cycle Inventory for Graduate Researchers — **Julian Silverman, Bala Subramaniam**

**5:10 Paper 565e:** Leadership Education for Engineers — **Dennis W. Hess**

**(566) Graphene 2-D Materials: Synthesis, Functions and Applications II**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 310

Lei Li, Chair  
Sanjay Behura, Co-Chair

**Sponsored by:** Carbon Nanomaterials

**3:30 Paper 566a:** Atomically-Precise Van Der Waals Heterostructures of Graphene and h-BN for 2D Circuits — **Sanjay Behura, Songwei Che, Chen Wang, Rousan Debbarma, Phong Nguyen, Michael R. Seacrist, Vikas Berry**

**3:45 Paper 566b:** Overcoming Micro-Silicon Particle Fracture within Graphene Cages for Stable Battery Anodes — **Yuzhang Li, Yi Cui**

**4:00 Paper 566c:** Patterning of Defect-Engineered Graphene Sheets Driven By Pore-Pore Interactions — **Ashish Kumar, Lin Du, Tam Nguyen, Dimitrios Maroudas**

**4:15 Paper 566d:** Synthesis and Applications of Magnetic Au-Ag- $\gamma$ - $\text{Fe}_2\text{O}_3$  Nanocomposites on Reduced Graphene Oxide — **Guangyu Lei, Jingwen Ma, Zhen Li, Xiaobin Fan, Wenchao Peng, Guoliang Zhang, Fengbao Zhang, Yang Li**

**4:30 Paper 566e:** Characterization of Lipid Dynamics and Structure on Epitaxial Graphene — **Megan Farrell, Maxwell Wetherington, Manish Shankla, Inseok Chae, Seong H. Kim, Aleksei Aksimentiev, Joshua Robinson, Manish Kumar**

**4:45 Paper 566f:** Detailed Characterization and Fabrication of 3D Printed Graphene/Polymer Structures for Heterojunction-Devices with MoS<sub>2</sub> and Other 2D Nanomaterials — **Deisy Arrington, Dylan Lynch, Vikas Berry**

**5:00 Paper 566g:** Laser Induced Graphene Conductive Films — **Patrick A. Johnson, Michael A. Seas, Joseph R. Murphy**

**5:15 Paper 566h:** Controlled Synthesis of Graphite Oxide: Formation Process, Oxidation Kinetics, and Optimized Conditions — **Chang Li, Liming Shen, Ningzhong Bao**

**5:30 Paper 566i:** WS<sub>2</sub>-Induced Enhanced Optical Absorption and Efficiency in Graphene/Silicon Heterojunction Photovoltaic Cells — **Rousan Debbarma, Sanjay Behura, Yu Wen, Songwei Che, Vikas Berry**

**(567) Highly Selective Separations with Membranes II**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 304

Stephen M. Ritchie, Chair  
D. Bhattacharyya, Co-Chair  
Milad R. Esfahani, Co-Chair  
Huanting Wang, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 567a:** Engineering the Nanochannels in Reduced Graphene Oxide Membranes for Dye Desalination — **Liang Huang, Haiqing Lin**

**3:51 Paper 567b:** Tuning Water Nanofiltration Performance of Few-Layered, Reduced Graphene Oxide Membranes By Oxygen Plasma — **Weiwei Xu, Fanglei Zhou, Miao Yu**

**4:12 Paper 567c:** Graphene Oxide Nanoplatelets Embedded Polyamide Thin Films for Water Desalination — **Mahsa Abbaszadeh, Santanu Kundu**

**4:33 Paper 567d:** Adhesion and Scaling Mechanism of Gypsum on the Commercial Microfiltration Membranes — **Yuxing Bai, Min Su**

**4:54 Paper 567e:** Permselective Transport of Organic Molecules in Perfluorosulfonic Acid Polymer Membranes for Personal Protective Equipment — **Anastasios Angelopoulos, Junchuan Fang**

**5:15 Paper 567f:** Phosphate-Functionalized Membranes for the Selective Sequestration of Uranium from Seawater — **Priyanka Suresh, Christine Duval**

**5:36 Paper 567g:** Highly Water Selective Mixed Matrix Membranes with UiO-66-Type MOFs in 6FDA-HAB/DABA Polyimide for Alcohol Dehydration Via Pervaporation — **Yiming Xu, Susilo Japip, Neal Tai-Shung Chung**

**(568) Integrative Systems Biology**

**Wednesday, Oct 31, 3:30 PM**

Westin Convention Center, Butler

Mark P. Brynildsen, Chair  
Jonathan L. Robinson, Co-Chair  
Peter St. John, Co-Chair

**Sponsored by:** Bioengineering

**3:30 Paper 568a:** A Quantitative Analysis of Integrin Activation on T Cell Homing — **Nicholas Anderson, Dooyoung Lee, Daniel A. Hammer**

**3:48 Paper 568b:** Simulating  $\text{Ca}^{2+}$  Signal Propagation in Exact 3D Reconstructions of Hepatic Lobules — **Rajanikanth Vadigepalli, Aalap Verma, Jan Hengstler, Jan Hoek, Babatunde A. Ogunnaik**

**4:06 Paper 568c:** Expecting the Unexpected: Synthesis Pathway-Host Incompatibility Due to Metabolic Network Disruption — **Sara Amin, Venkatesh EndalurGopinarayanan, Nikhil U. Nair, Soha Hassoun**

**4:24 Paper 568d:** Extending a Scalable Bayesian Metabolic Modeling Framework with Thermodynamic Constraints and Support for Transcriptional Regulation — **Jonathan Strutz, Peter St. John, Linda J. Broadbelt, Keith E.J. Tyo**

**4:42 Paper 568e:** Dynamic Sequence Specific Constraint-Based Modeling of *E. coli* Cell-Free Protein Synthesis — **Nicholas G. Horvath, Wei Dai, Michael Vilkhovoy, Jeffrey Varner**

**5:00 Paper 568f:** Towards a Metabolic and Expression Model of the Metabolically Versatile Bacterium *Rhodopseudomonas Palustris* — **Adil Alsiyabi, Rajib Saha**

**5:18 Paper 568g:** Towards a Predictive Synthetic Biology Enabled By Machine Learning and Automation — **Hector Garcia Martin**

**(569) KICHe-US Chapter Open Forum (Invited Talks)**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 331

Jaehun Chun, Chair  
You-Yeon Won, Co-Chair  
Tae-Sik Oh, Co-Chair

**Sponsored by:** International Committee

**3:30 Paper 569a:** NiMo-Ceria-Zirconia-Based Internal Reforming Solid Oxide Fuel Cell — **Su Ha**

**3:50 Paper 569b:** Micro-Solid Bubble Assembly for Ultralight, Strong, and Superelastic Materials — **Pil Jin Yoo**

**4:10 Paper 569c:** Electroactive Crystalline Phase Formation in Poly(vinylidene fluoride) Nanocomposite Films — **Jongwook Ha**

**4:30 Paper 569d:** Tailoring the Assembly of Electrode Materials Via Scalable Processes for High Capacity Li-Ion, Li-Sulfur, and Li-Air Batteries — **Yong Lak Joo**

**4:50 Paper 569e:** Integrated Synthesis-Capture Strategies for Viral Templated and Catalytically Active Palladium Nanoparticles Toward Multifunctional Membranes — **Hyunmin Yi**

**5:10 Paper 569f:** Effective Radiative Cooling with Photonic Random Media — **Sang Eon Han, Sarun Atiganyanun, John Plumley, Seok Jun Han, Kevin Hsu, Jacob Cytrynbaum, Thomas Peng, Sang M Han**

**(570) Microwave Chemistry for Fuel Conversion**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 321

Dushyant Shekhawat, Chair  
Jianli Hu, Co-Chair  
Christina Wildfire, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**3:30 Paper 570a:** Microwave Chemistry — **Dushyant Shekhawat, Mark Smith, Victor Abdelsayed, Christina Wildfire**

**3:48 Paper 570b:** Low-Temperature Microwave Plasma Conversion of Methane to Higher Hydrocarbons — **George Skoptsov, Kurt Zeller, Randy Vander Wal**

**4:06 Paper 570c:** Characterization of Products from Microwave-Assisted Pyrolysis of Biomass with Char Microwave Absorber — **Candice Ellison, Dorin Boldor**

**4:24 Paper 570d:** Catalyst Design for Microwave-Assisted Dry Reforming of Methane — **Christopher Marin, Douglas R. Kauffman**

**4:42 Paper 570e:** Techno-Economic Analysis of Direct Non-Oxidative Conversion of Shale Gas Via Non-Thermal Microwave (MW) Plasma Catalysis — **Chirag Mevawala, Jianli Hu, Debansu Bhattacharyya**

**5:00 Paper 570f:** Novel Microwave Assisted Ammonia Synthesis By Methane and Nitrogen Under Atmospheric Pressure — **Xinwei Bai, Sarojini Tiwari, Brandon Robinson, Jianli Hu**

**5:18 Paper 570g:** Spectroscopic and Microscopic Characterization of Nanographene Product By Microwave-Assisted Plasma-Mediated Methane Pyrolysis — **Randy Vander Wal, Madhu Singh, Arupnanda Sengupta, Kurt Zeller, George Skoptsov**

**5:36 Paper 570h:** Performance of Microwave-Assisted Catalysis for Production of Upgraded Pyrolysis Bio-Oil from Poplar Species in a Continuous-Flow System — **Dorin Boldor**, Cosmin Marculescu, Razvan N. State, Mariana Patrascu

#### (571) Modeling & Simulation of Complex Systems

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 316

Jerry Kaczur, Chair  
Yizu Zhu, Co-Chair

**Sponsored by:** Innovations of Green Process Engineering for Sustainable Energy and Environment

**3:30 Paper 571a:** Optimal Shale Gas Water Management: A Perspective from the Cooperative Games Theory — **Jose A. Caballero**, Viviani C. Onishi, Juan A. Reyes-Labarta, Alba Carrero-Parreño, Ruben Ruiz-Femenia, Raquel Salcedo-Díaz

**3:55 Paper 571b:** Spent Acid Recovery By Nanofiltration Membrane in Mining/Plating Industries – a Pilot Study — **Kang Hu, Bo Yan**

**4:20 Paper 571c:** Optimal Design and Dynamic Operation of MR Refrigeration System for Natural Gas Liquefaction Process — **Mozammel Mazumder**, Qiang Xu, Srinivas Palanki

**4:45 Paper 571d:** Insights from Thermodynamic System Analysis of Thermochemical Solids Looping Systems for Reforming and Combustion Applications — **Mandar Kathe**, Peter Sandvik, William K. Wang, Fanhe Kong, Liang-Shih Fan

**5:10 Paper 571e:** Improved Assessment of Personal Exposure to Chemicals Using Agent Based Modelling (ABM) Coupled with Multi-Sensors Networks — **Dimitrios Chapizanis**, Spyros Karakitsios, Dimosthenis Sarianni

**5:35 Paper 571f:** Small Scale H<sub>2</sub> Production Via Sorption Enhanced Chemical Looping Steam Reforming of Methane in an Adiabatic Packed Bed Reactor — **Syed Abbas**, Valerie Dupont, Tariq Mahmud

#### (572) Molecular Simulation of Adsorption II

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 305

Daniel W. Siderius, Chair  
Li-Chiang Lin, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**3:30 Paper 572a:** Solution-Phase Adsorption of Furan and Carboxylic Acid in Hierarchical Zeolites: Insights from Molecular Simulation — **Tyler R. Josephson**, Kristeen Esther Joseph, Paul J. Dauenhauer, J. Ilja Siepmann

**3:51 Break**

**4:12 Paper 572c:** First-Principles-Derived Force Fields for CH<sub>4</sub> Adsorption and Diffusion in Siliceous Zeolites — **Hanjun Fang**, Rohan Awati, Salah Eddine Boufelfel, Peter I. Ravikovitch, David S. Sholl

**4:33 Paper 572d:** Investigating High Pressure Methane Storage Using Lennard-Jones Crystals — **Alec R. Kaija**

**4:54 Paper 572e:** Formaldehyde Adsorption Performance of Selected Metal-Organic Frameworks from High-Throughput Computational Screening — **Wei Li**

**5:15 Break**

**5:36 Paper 572g:** Modeling and Simulation of Multicomponent Adsorption Columns — **Gerassimos Orkoulas**, Dipendu Saha

#### (573) Nanoscale Structure in Polymers

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 327

Shrayesh Patel, Chair  
Ju-Won Jeon, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 573a:** Manufacturing Functional Membranes from Nanostructured Polymers — **William A. Phillip**

**4:00 Paper 573b:** Electron Tomography Reveals Details of the Internal Microstructure of Desalination Membranes — **Tyler E. Culp**, Yue-xiao Shen, Michael Geitner, Mou Paul, Abhishek Roy, Michael Behr, Steve Rosenberg, Junsu Gu, Manish Kumar, Enrique D. Gomez

**4:15 Paper 573c:** Synthesis and Self-Assembly of a New High- $\chi$  Block Copolymer: Ptbs-b-Phema — **Caleb Breaux**, Brandon L. Sharp, Haibo Li, Benjamin Li, Mark Neisser, Clifford L. Henderson

**4:30 Paper 573d:** Assembly and Photoswitching Dynamics in Nanostructured Polymer Thin Films Revealed By Single-Molecule Super-Resolution Microscopy — **Muzhou Wang**, Zhe Qiang, Kevin Shebek

**4:45 Paper 573e:** Nanostructured Polymer Gels and Brushes Via 2 Color Interference Lithography — **Harikrishnan Vijayamohanan**, Edmund Palermo, Chaitanya Ullal

**5:00 Break**

**5:30 Paper 573h:** Effect of Curing Bath Conditions on the Morphology of Porous Hollow Poly(High Internal Phase Emulsion) Fibers — **Xuehui Gong**, Donald L. Feke, Ica Manas-Zloczower

**5:45 Paper 573i:** Geometry and Composition of Soft Polymer Films Embedded with Nanoparticles Enhance Rates for Optothermal Heat Dissipation — **D. Keith Roper**, Keith Berry, Jeremy Dunklin

#### (574) Nanostructured Thin Films

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 329

Wei Fan, Chair  
Seok-Jhin Kim, Co-Chair  
Jong Suk Lee, Co-Chair

**Sponsored by:** Inorganic Materials

**3:30 Paper 574a:** Multi-Scale Engineering of Polyimide-Derived Carbon Molecular Sieves — **Megha Sharma**, Mark A. Snyder

**3:48 Paper 574b:** Mesoscale Thermal Transformation Kinetics and Mechanism for the Synthesis of SiO<sub>2</sub>-TiO<sub>2</sub> Mixed Thin Films with Sub-3 Nanometer Vertical Pore Channels — **M. Arif Khan**, Rami Ghanim, Joshua Garay, Aniruddha Shirodkar, Yuxin He, Mahsa Moradipour, Barbara L. Knutson, Stephen E. Rankin

**4:06 Paper 574c:** Controlling Sulfur Corrosion of Pd-Cu Hydrogen Separation Membranes with Ultra-Thin Metal Films — **Casey O'Brien**

**4:24 Paper 574d:** Formation of Ordered Nanostructure Patterns on Surfaces of Biaxially Stressed Thin Films — **Lin Du**, Ashish Kumar, Dimitrios Maroudas

**4:42 Paper 574e:** Atmospheric-Pressure Plasma Patterning and Reduction of Metal-Ion Containing Polymer Films to Fabricate Stretchable Electrically Conducting Features — **Souvik Ghosh**, R. Mohan Sankaran

**5:00 Paper 574f:** Group Contribution Method for Atomic Layer Deposition Based on Adsorbate Solid Solution Theory for Computer Aided Design of Novel Materials and Nanostructures — **Mina Shahmohammadi**, Rajib Mukherjee, Christos G. Takoudis, Urmila M. Diwekar

**5:18 Paper 574g:** Understanding the Formation and Pyrolysis of Metal Thiolate Complexes for Solution-Processed Thin Film Photovoltaics — **David Rokke**, Swapnil Dattatray Deshmukh, Xin Zhao, Rakesh Agrawal

**5:36 Paper 574h:** Investigation of Electrical and Optical Properties of Indium Oxide Thin-Films Prepared By Atomic Layer Deposition Using Trimethylindium and Ozone Precursors — **Hossein Salami**, Alan Uy, Vivek Dwivedi, Raymond A. Adomaitis

#### (575) Nanotechnology for Biotechnology and Pharmaceuticals II

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 311

Kevin J. Cash, Chair  
Margaret Bennewitz, Co-Chair

**Sponsored by:** Bionanotechnology

**3:30 Paper 575a:** Invited Speaker: Lipophilically-Functionalized Porous Silica Nanoparticles for Acoustic Imaging and Site-Specific Therapy — **Andrew P. Goodwin**

**4:10 Paper 575b:** Nanoparticles for Combination Chemotherapy — **Shani Levit**, Christina Tang

**4:28 Paper 575c:** Co-Loading of Hydrophilic and Lipophilic Therapeutics through Equilibration within Temperature Sensitive Liposomes — **Shrishti Singh**, Steven Roberts, Nitin Agrawal

**4:46 Paper 575d:** Novel Nano Biotechnology Approaches for Treating Intracellular Bacterial Infections — **Kristen Eller**, Max Levy, Jocelyn Campos, Thomas Aunins, Stephanie J. Bryant, Prashant Nagpal, Anushree Chatterjee

**5:04 Paper 575e:** A Virus-Free Fe<sub>3</sub>O<sub>4</sub> Nanoparticle-Based H7N9 Influenza Vaccine — **Alan Roberto Márquez-Ipiña**, Grissel Trujillo-de Santiago, María de los Angeles De Santiago-Miramontes, Mario Moisés Alvarez



**5:22 Paper 575f:** Engineering Lipid Nanoparticles to Mitigate Oxidative Stress in Stem Cell Transplant Therapy — *Rashi Porwal, Stephen L. Hayward, Srivatsan Kidambi*

**5:40 Paper 575g:** Sugar-Guided Organ and Cellular Targeting of PAMAM Dendrimers — *Joshua E. Porterfield, Rishi Sharma, Anjali Sharma, Kevin Liaw, Elizabeth Smith, Sujatha Kannan, Rangaramanujam Kannan*

#### (576) New Methods in Polymer Modeling

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 326

Douglas Tree, Chair  
Jian Qin, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 576a:** Role of Nucleoid Associated Proteins in Stabilizing DNA Supercoils — *Katelyn Dahlke, Charles E. Sing*

**3:45 Paper 576b:** A Modeling Approach to Understanding and Improving Thermal Comfort in Polyurethane Mattress Foams — *Laura J. Dietsche, Douglas Brune, Wenbo Xu, Kaoru Aou, Rajat Duggal*

**4:00 Paper 576c:** Mesoscale Modeling of Plant Cell Walls and Understanding Their Mechanics during Cell Growth — *Sriramvignesh Mani, Fikret Aydin, Gregory A. Voth*

**4:15 Paper 576d:** Multiscale Modeling of Hyperelastic Deformation and Related Microstructural Properties of Random Cross-Linked Elastomers — *Shashank Mishra, Suryanama Chauhe, Soumyadip Maiti, Beena Rai*

**4:30 Paper 576e:** Molecular Simulation of Micellar Chain Exchange Kinetics of Asymmetric B<sub>2</sub>AB<sub>2</sub> Linear Triblock and AB<sub>2</sub>B<sub>2</sub> branched Triblock Copolymers — *Andrew Peters, Timothy P. Lodge*

**4:45 Paper 576f:** Influence of Hydrodynamic Interactions on Stratification in Drying Mixtures — *Antonia Statt, Michael P. Howard, Athanassios Z. Panagiotopoulos*

**5:00 Paper 576g:** Optimization Methods for Polymerization Processes with Detailed Microstructural Quality Indices — *Yannan Ma, Xi Chen, Lorenz T. Biegler*

**5:15 Paper 576h:** *In silico* Exploration of Polyimides with High Index of Refraction Using Molecular Modeling and High-Throughput Screening — *Mohammad Atif Faiz Afzal, Chong Cheng, Johannes Hachmann*

**5:30 Paper 576i:** Synthesis and Self-Assembly of the Low- $\chi$  Block Copolymer Ptb<sub>s</sub>-b-Ppma — *Caleb Breaux, Haibo Li, Benjamin Li, Mark Neisser, Clifford L. Henderson*

**5:45 Paper 576j:** Deformation of Linear and Short Chain Branched Semicrystalline Polyethylene — *Raghavan Ranganathan, Vaibhaw Kumar, George Rodriguez, Andy H Tsou, Gregory C. Rutledge*

#### (577) North American Mixing Forum Award Session (Invited Talks)

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 334

David S. Dickey, Chair  
Richard K. Grenville, Co-Chair

**Sponsored by:** North American Mixing Forum

**3:30 Paper 577a:** NAMF Award Lecture: Lessons from Mixing Studies Involving Bacteria, Fungi and Chocolate — *Enrique Galindo*

#### (578) Novel Nanoparticles and Nanostructured Materials for Environmental Applications

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 413

Satish Nune, Chair  
Alan W. Weimer, Co-Chair  
Xing Yangchuan, Co-Chair

**Sponsored by:** Nanoparticles

**3:30 Paper 578a:** A Novel Semiconductor Nanofiber with Superb Charge Conductivity for Energy and Environmental Applications — *Wallace Woon-Fong Leung*

**4:00 Paper 578b:** Bioinspired Nanomaterials for Environmental Remediation — *Siddharth V. Patwardhan, Lorraine T Gibson*

**4:25 Paper 578c:** Encapsulation of Nanoscale Hybrid Materials for Innovative CO<sub>2</sub> capture: NOHMs and MOFs — *Ming Gao, Wei Yu, Ah-Hyung Alissa Park*

**4:50 Paper 578d:** Nanostructured Au/Organoclay Materials for Methylmercury Adsorption — *Kae Fink, Shu Yang, Andrea Chica, William P. Johnson, Michael M. Nigra*

**5:15 Paper 578e:** Surface Modification of a Mxene with Silane Coupling Agents — *Hossein Riaz, Ahmad Arabi Shamsabadi, Babak Anasori, Yuri Gogotsi, Masoud Soroush*

**5:40 Paper 578f:** Flame Synthesis of Crumpled Graphene Nanostructures Decorated with Multicomponent Metal Nanoparticles — *Mohammad Moein Mohammadi, Santosh Srivatsa Gunturi, Shikuan Shao, Raymond Buchner, Mark T. Swihart*

#### (579) NSF Workshop II: Proposal Writing and Discussions with Program Managers

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 411

Ram B. Gupta, Chair  
Richard Dickinson, Co-Chair

**Sponsored by:** Career Guidance Committee Liaison

**3:30 Paper 579a:** Proposal Writing Tutorial — *William L. Olbricht*

**4:30 Paper 579b:** Interactive Breakout Panels — *Carole Read, Steven Peretti, Bruce Hamilton, Susan Muller, T. J. Mountziaris*

#### (580) Nucleation and Growth II

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 302

Venkateswarlu Bhamidi, Chair  
Meenesh R. Singh, Co-Chair

**Sponsored by:** Crystallization and Evaporation

**3:30** Welcoming Remarks

**3:35 Paper 580a:** Integrated Kinetic Monte-Carlo Method to Find Face Specific Growth Rates — *James Fell, Anish V. Dighe, Meenesh R. Singh*

**3:55 Paper 580b:** High Aspect Ratio Metal Organic Framework Synthesis Using Microfluidic Devices — *Stephanie Guthrie, Luke Huelsenbeck, Walter Varhue, Armita Salahi, Nathan Swami, Gaurav Giri*

**4:15 Paper 580c:** Towards Modelling Facet-Specific Impurity Incorporation Rates Using Molecular Dynamics Simulations – a Case Study on the Urea/Biuret/Water System — *Thomas Brindley, Sendhil Poornachary, Reginald Tan, Thomas Vetter*

**4:35 Paper 580d:** Designing Inhibitors of Mineral Scale: A New Platform Based on Cooperative Microfluidic and Computational Assays — *Ricardo D. Sosa, Xi Geng, Jeremy C. Palmer, Michael A. Reynolds, Jacinta C. Conrad, Jeffrey D. Rimer*

**4:55 Paper 580e:** Secondary Nucleation and Growth Kinetics of Aluminum Hydroxide Crystallization from Potassium Aluminate Solution Using FBRM — *Jin Xue, Cheng-Lin Liu, Mengjie Luo, You-Fa Jiang, Ping Li, Jianguo Yu, Sohrab Rohani*

**5:15 Paper 580f:** Crystallization Behaviors of Lithium Carbonate in Strong Alkaline Solution: Solubility, Nucleation Mechanism, and Particle Size Control — *You-Fa Jiang, Cheng-Lin Liu, Jin Xue, Mengjie Luo, Ping Li, Jianguo Yu*

**5:35 Paper 580g:** Study on Crystallization Kinetics of Calcium Carbonate By FBRM in-Situ Monitoring — *Yingying Zhao*

#### (581) Polymer Phase Change and Assembly

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 333

Ying Diao, Chair  
Xue (Ida) Chen, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 581a:** Towards Molecular Design of Conjugated Polymers: Glass Transition, Liquid Crystal Phases, and Entanglements — *Enrique D. Gomez*

**4:00 Paper 581b:** Understanding Crystallization of Oriented Domains in Solution Printed Organic Semiconductor Thin Films — *Ge Qu, Ying Diao*

**4:15 Paper 581c:** Role of Phase Morphology on the Electronic and Structural Landscape of Organic Semiconductors — *Aditi Khirbat, Ilaria Bargigia, Giovanni M. Matrone, Artem Levitski, Mark D. Losego, Carlos Silva, Gitti Frey, Natalie Stingelin*

**4:30 Paper 581d:** Controlling Self-Assembly for Enhanced Interconnection in Conjugated Polymer Networks — *Michael McBride, Guillermo Bacardi, Aarti Mathur, Elsa Reichmanis, Martha A. Grover*

**4:45 Paper 581e:** Bio-Inspired Dynamic Templates for Directing Multi-Scale Assembly of Polymer Semiconductors — *Erfan Mohammadi, Ying Diao*

**5:00 Paper 581f:** Self-Assembly of Bottlebrush and Star-like Copolymer Architectures in Solution: A Coarse-Grained Molecular Simulation Study — *Michiel G. Wessels, Arthi Jayaraman*

**5:15 Paper 581g:** Analyzing the Effects of the Solution Casting Process on Block Copolymer Microphase Separation Kinetics Using *in-Situ* x-Ray Scattering — **Alicia R. Pape, Ninad Dixit, Rui Zhang, Louis Madsen, John A. Pople, Stephen M. Martin**

**5:30 Paper 581h:** Thermodynamic Manipulation of Polymerization Induced Phase Separation: Influence of Entropic Versus Enthalpic Driving Forces — **Caroline Szczepanski, John M. Torkelson**

**5:45 Paper 581i:** Simultaneous in-Film Polymerization with Self-Assembly for on-Demand Manipulation of Polymer Functionality — **Zhe Qiang, Sahil Akolawala, Kevin Shebek, Muzhou Wang**

**(582) Polymer Reaction Engineering**  
**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 324

Iman Noshadi, Chair  
Christian Pester, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 582a:** Reaction Kinetics of Moisture-Reactive Materials for Experimental Validation of a Model for Water Vapor Reaction, Sorption, and Diffusion in Polymers — **Jennifer M. Knipe, Hom Sharma, Justin Sirrine, April M. Sawvel, Yunwei Sun, Elizabeth Glascoe**

**4:00 Paper 582b:** Advances in Organophotocatalysis: Reaction Mechanisms and Applications in Organic and Polymer Synthesis — **Alan Aguirre-Soto**

**4:15 Paper 582c:** Synthesis and Characterization of Cyclic Poly(vinylmethylsiloxane)-b-Poly(methyl methacrylate)s — **Baraka S Lwoya, Md Fakar Uddin, Sourav Chatterjee, Saeed Behzadinasab, Julie N. L. Albert**

**4:30 Paper 582d:** Controlled Synthesis of Hyperbranched Polymers Via Semibatch Atom Transfer Radical Copolymerization — **Mingjiang Zhong, Feng Li, Mengxue Cao, Yujun Feng**

**4:45 Paper 582e:** Tuning Compositional Drift in the Bulk Living Copolymerization of Styrene and Isoprene — **Bryan S. Beckingham, Sneha B Chakrapani**

**5:00 Paper 582f:** Catalytic Emulsion Polymerization of Ethylene — **Damien Guironnet**

**5:15 Paper 582g:** Peptide Hydrolysis and the Prebiotic Origin of Functional Peptides — **Yi Sun, Martha A. Grover, Charles Liotta**

**5:30 Paper 582h:** D-Optimal Estimation of Polyolefin Polymerization Rate Constants Using Experimental Residence Time Studies in Industrial Pilot Plant Equipment — **Thomas W. Karjala, Brian Kolthammer, Min Zhang, Pradeep Jain**

**5:45 Paper 582i:** Tailoring Uniform Copolymer Composition Distribution Via Policy II RAFT Solution Copolymerization of Styrene and Butyl Acrylate — **Jie Jiang, Wen-Jun Wang, Shiping Zhu, Bo-Geng Li**

**(583) Process Intensification through Process Systems Engineering**

**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, 409

M. M. Faruque Hasan, Chair  
Ankur Kumar, Co-Chair

**Sponsored by:** Systems and Process Design

**3:30 Paper 583a:** A Reactive Distillation Optimization Model for Low- and High-Temperature Fischer-Tropsch Syntheses for Multiphase Product Recovery — **Yanyan Hu, Naian He, Yizu Zhang, Cornelius Mduduzi Masuku, Lorenz T. Biegler**

**3:49 Paper 583b:** Design and Intensification of Sorption-Enhanced Reaction Processes for Methanol Production — **Akhil Arora, Shachit S. Iyer, Ishan Bajaj, M. M. Faruque Hasan**

**4:08 Paper 583c:** Comparison of Adsorptive Separation Performance of a Hollow Fiber Bed and a Packed Bed: A Modeling Study Using Zeolite 13X and a Mixture of Propylene and Propane — **Trisha Sen, Yoshiaki Kawajiri, Matthew J. Realff**

**4:27 Paper 583d:** Towards a Systematic Process Intensification Framework for Advanced Distillation Systems — **Yuhe Tian, M. Sam Mannan, Efstratios N. Pistikopoulos**

**4:46 Paper 583e:** An MILP-Based Operability Approach for Process Design, Intensification and Modularity of Nonlinear and High-Dimensional Energy Systems — **Vitor Gazzaneo, Fernando V. Lima**

**5:05 Paper 583f:** Compact, Nonsmooth Operators for Single-Component Mass and Water Integration — **Caroline Nielsen, Paul I. Barton**

**5:24 Paper 583g:** Optimal Mass Exchanger Network Synthesis Using a 2-Step Hybrid Algorithm Including Packed Column Design — **Michael Short, Lorenz T. Biegler, Adeniyi J. Isafiade**

**5:43 Paper 583h:** Mathematical Optimization of Sustainable Water Desalination Processes Using Directional Solvent Extraction — **Alejandro Garciadiego, Tengfei Luo, Alexander W. Dowling**

**(584) Process Monitoring & Fault Detection**

**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, 410

Zhenyu Wang, Chair  
Donald J. Chmielewski, Co-Chair

**Sponsored by:** Data and Information Systems

**3:30 Paper 584a:** System Decomposition for Distributed Multivariate Statistical Process Monitoring — **Shaaz Khatib, Prodomos Daoutidis, Ali Almansoori**

**3:45 Paper 584b:** Transfer Entropy-Based Dynamic Causal Maps Generation for Fault Diagnosis in Systems with Cycles — **Resmi Suresh, Abhishek Sivaram, Venkat Venkatasubramanian**

**4:00 Paper 584c:** Efficient Process Monitoring and Causality Analysis of Processes Via the Integrated Use of the Graphical Lasso and Markov Random Fields Modeling — **Changsoo Kim, Hodong Lee, Wonbo Lee**

**4:15 Paper 584d:** Transfer Learning Method for Chemical Plant Fault Diagnosis — **Junyao Xie, Stevan Dubljevic**

**4:30 Paper 584e:** Multi-Class Classification of Process Faults Using Nonlinear Support Vector Machine Based Feature Selection Algorithm — **Melis Onel, Efstratios N. Pistikopoulos**

**4:45 Paper 584f:** In Situ FT-IR Quantitative Analysis of Amine Concentration and CO<sub>2</sub> Loading Amount in Mixture Solvent Using Deep Neural Network — **Yo Sung Yoon, Jay H. Lee**

**5:00 Paper 584g:** Deep Learning for Pyrolysis Reactor Monitoring: From Thermal Imaging Towards Smart Monitoring System — **Wenbo Zhu, Jose A. Romagnoli**

**5:15 Paper 584h:** Model-Based Stochastic Fault Detection and Diagnosis of Lithium-Ion Batteries — **Jeongeun Son, Yuncheng Du**

**5:30 Paper 584i:** Implementation of Model-Predictive Safety Systems to Detect Predictively Operation Hazards in Non-Minimum-Phase Processes — **Masoud Soroush, Jeffrey E. Arbogast, Warren D. Seider, Ahmad Arabi Shamsabadi**

**(585) Protein Engineering for Therapeutics**

**Wednesday, Oct 31, 3:30 PM**  
Westin Convention Center, Westmoreland East

Yongku Cho, Chair  
Robert Pantazes, Co-Chair

**Sponsored by:** Bioengineering

**3:30 Paper 585a:** Structure-Guided Molecular Engineering of a VEGF Antagonist to Treat Retinal Eye Diseases — **Jamie B. Spangler**

**3:48 Paper 585b:** Probing the Conformation and Phospho-Specificity of Anti-Tau Antibodies Using Yeast Surface Display — **Shiyao Wang, Yongku Cho**

**4:06 Paper 585c:** Novel Protein Engineered for the Treatment of Malaria — **Patrick McKernan, Roger Harrison**

**4:24 Paper 585d:** A High-Throughput *in Vitro* compartmentalization (IVC) Directed Evolution Platform for Engineering Protease Substrate Specificity — **Carl A. Denard, Zachary Bennett, Joseph Taft, Joseph DeSautelle, Rasha Yaghi, Brent L. Iverson**

**4:42 Paper 585e:** Exploiting Reactive Chemical Functionality in Antibodies to Introduce Metalloproteinase-Targeting Functional Groups — **Laura B. Quinto, Jessica T. Stieglitz, Gregory I. Berumen, Haixing P. Kehoe, James Van Deventer**

**5:00 Paper 585f:** Optmaven-2.0: A Fast Protocol for *de novo* Design of Antibody Variable Region Against Aspecific Antigen Epitope — **Ratul Chowdhury, Matthew F. Allan, Costas D. Maranas**

**5:18 Paper 585g:** Biomolecular Engineering for Non-Invasive Imaging and Control of Cellular Function — **Mikhail G. Shapiro**

**(587) Survey Results and Best Practices: Thermodynamics (Invited Talks)**  
**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 405

Margot Vigeant, Chair  
 Kevin Dahm, Co-Chair  
 David L. Silverstein, Co-Chair

**Sponsored by:** Undergraduate Education

**3:30** Introductory Remarks

**3:35 Paper 587a:** How We Teach: Chemical Engineering Thermodynamics — *David L. Silverstein, Margot A.-S. Vigeant, Kevin Dahm, Lucas J. Landherr, Jennifer Cole, Laura Ford*

**4:05 Paper 587b:** Perspectives on Thermodynamics Instruction — *Donald P. Visco Jr., Kevin Dahm*

**4:50** Discussion

**(588) The Industrial Fluid Properties Simulation Challenge**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 308

Jonathan Moore, Chair  
 Daniel W. Siderius, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**3:30 Paper 588a:** Beyond United-Atom Lennard-Jones: Reliable Prediction of High Pressure Viscosities — *Richard A. Messerly, Andrei Kazakov, J. Richard Elliott Jr., S. Mostafa Razavi*

**4:00 Paper 588b:** Prediction of the Viscosity-Pressure Relation Using Nonequilibrium Molecular Dynamics — *Irais Valencia-Jaime, Brittany Gonzalez, Solene Bechelli, Steve Groven, Caroline Desgranges, Jerome Delhommelle*

**4:30 Paper 588c:** Results of the Tenth Industrial Fluid Properties Simulation Challenge: Pressure-Dependence of Viscosity for a Short, Branched Alkane — *Scott Bair*

**(589) Thermodynamics at the Nanoscale**

**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 307

Amish Patel, Chair  
 Sapna Sarupria, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**3:30 Paper 589a:** Invited Talk: Role of Interfacial Water in Adhesion and Friction — *Ali Dhinojwala*

**4:00 Paper 589b:** Directly Measuring the Diamond Nucleation Landscape to Test Classical Nucleation Theory — *Matthew A. Gebbie, Nicholas A. Melosh*

**4:20 Paper 589c:** Carbon in Liquid Silicon: Diffusion, Solubility, and Silicon-Carbide Nucleation — *Abdullah Alateeqi, Jinping Luo, Lijun Liu, Talid Sinno*

**4:40 Paper 589d:** How the Solvation of Flexible Solutes Influences Their Conformations — *Debdas Dhabal, Zhitong Jiang, Amish Patel*

**5:00 Paper 589e:** Invited Talk: Using PRISM Theory and Molecular Simulations to Link Polymer Architecture to Structure and Thermodynamics at the Nanoscale in Polymer Solutions — *Arthi Jayaraman*

**5:30 Paper 589f:** Time-Temperature Superposition for Integration of Atomistic Simulations with Experiment for Thermomechanical Properties of Cross-Linked Epoxy — *Ketan S. Khare, Frederick R. Phelan Jr.*

**(590) Tribute to Jacques L. Zakin: Scholar, Teacher and Mentor III (Invited Talks)**

**Wednesday, Oct 31, 3:30 PM**

Omni William Penn Hotel, Conference Center A

Liang-Shih Fan, Chair  
 Bhavik R. Bakshi, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 590a:** Polyelectrolytes in Multivalent Ionic Media: New Physics and New Materials — *Matthew V. Tirrell*

**3:55 Paper 590b:** Stimuli-responsive Surfactant Self-assembly — *Nicholas L. Abbott*

**4:20 Paper 590c:** Photoreological Fluids Based on Surfactants and Polymers: Applications in Turbulent Drag Reduction and Microfluidic Flow Control — *Srinivasa R. Raghavan*

**4:45 Paper 590d:** Type B Drag Reduction Fundamentals — *Preetinder S. Virk*

**5:10 Paper 590e:** Flow-assisted Polymer Degradation in Turbulent Boundary Layers — *Brian R. Elbing*

**5:35 Paper 590f:** Dynamics of Adsorption of Rhamnolipid Biosurfactants at Air/water and Oil/water Interfaces — *Stephanie Kirby, Shelley L. Anna, Lynn Walker*

**(591) USA-China Progress in Biomass Conversion Technology III**  
**Wednesday, Oct 31, 3:30 PM**

David L. Lawrence Convention Center, 325

Yulin Deng, Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**3:30 Paper 591a:** Production of 5-Hydroxymethylfurfural from Glucose Using a Resin Solid Acid — *Tingwei Zhang, Wenzhi Li*

**3:55 Paper 591e:** Low Temperature and High Efficiency Biomass Fuel Cell and Bio-Hydrogen Production — *Yulin Deng*

**4:20 Paper 591c:** Nano Core-Shell Structured ZSM-5@Mesoporous Silica for Catalytic Co-Cracking Phenolic Bio-Oil Model Compounds and Ethanol to Aromatics — *Wenbo Wang, Simin Li, Yi Yang, Shuang Xue, Kongyu Lu, Zhongyang Luo*

**4:45 Paper 591d:** Experimental Research on Wet-Press Molding Features and Microstructure Change of Wheat Straw — *Jianjun Hu, Gang Li, Chao He, Yi Wang*

**(592) Rapid Fire Session: Environmental Division**

**Wednesday, Oct 31, 4:45 PM**

David L. Lawrence Convention Center, 319

Debalina Sengupta, Chair  
 Sage R. Hiibel, Co-Chair  
 Jeffrey Seay, Co-Chair

**Sponsored by:** Environmental Division

**4:45** Break

**4:50 Paper 592b:** Optimization Study for Wet Air Oxidation of Ethylene Plant — *Shehzada Khurram*

**4:55 Paper 592c:** Microbially-Mediated Moisture Retention in Emulated Soil Micromodels — *Yi-Syuan Guo, Jessica M. Furrer, Daniel J. Gage, Yongku Cho, Leslie M. Shor*

**5:00 Paper 592d:** Green Synthesis of Nano Iron Carbide: Preparation, Characterization and Application for Removal of Phosphate from Aqueous Solutions — *Rabie Farag, Dr. Maha M. El-Shafei, Ahmed S. Mahmoud, Mohamed K. Mostafa, Robert W. Peters*

**5:05 Paper 592e:** Extraction of Chlorophenols from Wastewater Using Ionic Liquids As Green Solvents — *Inas M. Alnashef, Reyihangu Sulaiman, Shadi Wajih Hasan*

**5:10 Paper 592f:** Ecohydrological Management and Valuation Insights of Ecosystem Services in Salt Lakes through Advanced Dynamic Optimisation Strategies — *Amira Siniscalchi, Carla V. Garcia Prieto, Eduardo Gomez, Ariel Raniolo, Rubén José Lara, María Soledad Diaz*

**5:15 Paper 592g:** From Thermopower Waves to Asymmetric Chemical Doping – New Concepts in Energy Storage and Generation Using Molecular Interactions with Single-Walled Carbon Nanotubes — *Albert Tianxiang Liu, Sayalee G. Mahajan, Yuichiro Kunai, Anton L. Cottrill, Michael Strano*

**(593) Poster Session: NH3 Energy+ Technologies**

**Wednesday, Oct 31, 5:30 PM**

David L. Lawrence Convention Center, 318

Trevor Brown, Co-Chair

**Sponsored by:** NH3 Energy+

**Paper 593a:** My Demonstration Renewable Energy System — *Jay Schmucke*

**Paper 593e:** Chemical Kinetic Modelling of Ammonia-Hydrogen-Air Premixed Flames — *Rodolfo Rocha, Mário Costa, Xue-Song Bai*

**Paper 593f:** Vanadium As a Potential Catalytic Membrane Reactor Material for NH3 Production — *Simona Liguori, Jennifer Wilcox*

**(594) Adsorbent Materials**  
**Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 309

Dipendu Saha, Chair  
 Jian Liu, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**8:00 Paper 594a:** Electrospun Nanoparticle/Nanofiber Composites (ENNCs) As New Core-Shell Adsorbent Materials — *Bin Mu*



**8:20 Paper 594b:** The Structure-Property Relationships of Metal-Organic Frameworks for Ethylene/Ethane Separation — **Yutao Gong**, Krista S. Walton

**8:40 Paper 594c:** Enhanced SF6 adsorption Kinetics By Hierarchically Structured Nanoporous Materials — **Chong Yang Chuah**, Tae-Hyun Bae

**9:00 Paper 594d:** Development of Small-Pore Rho Zeolites for Gas Separation Applications — **Elizabeth Seibel**, Magdalena M. Lozinska, Paul A. Wright, Shubra Bhadra, William Casteel Jr., Garret Lau, Erin Sorensen, Roger D. Whitley

**9:20 Paper 594e:** Molecular Blends of Methylated-Poly(ethylenimine) and Amorphous Porous Organic Cages for SO<sub>2</sub> Adsorption — **Guanghui Zhu**, Christopher W. Jones, Ryan Lively

**9:40 Paper 594f:** Acetic Acid Extraction Using Amine Grafted OMS: Effects Due to Degree of Amine Methylation — **Peter Miller**, Daniel F. Shantz

**10:00 Paper 594g:** Low Temperature Synthesis of Magnetic Carbonaceous Materials Coated with Silica for the Effective Adsorption of Methylene Blue for Aqueous Solution — **Reshma Babu**, Hemant Mittal, Saeed Alhassan

**(595) Advanced Treatment for Water Reuse and Recycling I**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 319

Jeffrey McCutcheon, Chair  
Sage R. Hilbel, Co-Chair

**Sponsored by:** Water

**8:00 Paper 595a:** Fabrication of Loose Inner-Selective Polyethersulfone (PES) Hollow Fibers By One-Step Spinning Process for Nanofiltration (NF) of Textile Dyes — **Jie Gao**, Zhiwei Thong, Kaiyu Wang, Neal Tai-Shung Chung

**8:15 Paper 595b:** Design of a Molecular-Recognition Material for Capture and Release of Phosphate — **Whitney Fowler**, Juan J. de Pablo, Matthew V. Tirrell

**8:30 Paper 595c:** Reactive Membranes for the Degradation of Emerging Wastewater Contaminants — **Michael Geitner**, Moon Son, Boya Xiong, Wulin Yang, Darrell Velegol, Bruce E. Logan, Manish Kumar

**8:45 Paper 595d:** Electrochemically Mediated Regeneration of Ionic Liquids (EMRIL) for Heavy Metal Removal and Water Disinfection — **Sahag Voskian**, Paul Brown, Krzysztof P. Rajczykowski, Cesar de la Fuente-Nunez, T. Alan Hatton

**9:00 Paper 595e:** A Polypyrrole-Based Asymmetric System for Electrochemically Mediated Separations of Organics from Water — **Yinying Ren**, Xianwen Mao, T. Alan Hatton

**9:15 Paper 595f:** Polyaniline Nanofiber Electrodes for Reversible Capture and Release of Mercury(II) — **Yoonseob Kim**, Timothy Swager

**9:30 Paper 595g:** Cyanide Recovery from Barren Solution Using UV Photodissociation and Gas-Filled Membrane Technology — **Kashinath Banerjee**, Herve Buisson, Tapas Das

**(596) Advances in Fluid Particle Separations**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 301

Isaac Gamwo, Chair  
Badie Morsi, Co-Chair

**Sponsored by:** Fluid-Particle Separations

**8:00 Paper 596a:** Modeling of the Flow Dynamics through Incompressible Porous Media in Solid-Liquid Filtration — **Siying Zhang**, Joseph J. McCarthy

**8:25 Paper 596b:** Two-Drop Model of Depth Coalescing Filter Performance — **Seyedeh Neda Mehdizadeh**, George G. Chase

**8:50 Paper 596c:** Cake Filtration of Catalyst Materials — **Zainab Abd Al-Jaleel**, Tulsi Char, Bill Borghard, Nina C. Shapley

**9:15 Paper 596d:** The Role of Pore Structure and Chemistry on Particle Deposition during Membrane Filtration — **Mirco Sorci**, Corey C. Woodcock, Joel L. Plawsky, Georges Belfort

**(597) Advances in Metabolic Engineering of Non-Model Organisms**

**Thursday, Nov 1, 8:00 AM**  
Westin Convention Center, Westmoreland East

Nanette R. Boyle, Chair  
Robert Jinkerson, Co-Chair  
Arul Varman, Co-Chair  
Hsien-Chung Tseng, Co-Chair

**Sponsored by:** Bioengineering

**8:00 Paper 597a:** Balancing Kinetic and Thermodynamic Barriers to Isomerization Catalysis in Probiotic *Lactobacillus Plantarum* — **Josef Bober**, Nikhil U. Nair

**8:18 Paper 597b:** Genome Engineering of *Lactococcus Lactis* for Pyrolytic Sugar Usage By a Cryptic Native Transformation Pathway — **Samuel Rothstein**, Swastik Sen, Thomas J. Mansell

**8:36 Paper 597c:** Improving C<sub>4</sub> to C<sub>2</sub> Ratio for n-Butanol Production in Mixotrophic Fermentation By Engineered *Clostridium Carboxidivorans* — **Tianyi Chen**, Chi Cheng, Teng Bao, S.T. Yang

**8:54 Paper 597d:** Utilizing Native Metabolic Pathways in *Deinococcus Radiodurans* for Metallic Nanoparticle Biosynthesis — **Angela Chen**, Benjamin K. Keltz, Lydia M. Contreras

**9:12 Paper 597e:** Synthetic Biology Tools Development and Metabolic Engineering of *Yarrowia Lipolytica* for Producing Lipid-Based Chemicals — **Xiaochao Xiong**, Rishikesh Ghogare, Shulin Chen

**9:30 Paper 597f:** Discovery of Metabolic Pathways for Conversion of Lignin-Derived Phenolics to Lipids in *Cutaneotrichosporon Oleaginosus* — **Allison Yaguchi**, Michael Spagnuolo, Alana Robinson, Erin Mihealsick, Mark Blenner

**9:48 Paper 597g:** *Elucidating Core Design Principles to Engineer Nonconventional Yeasts As Novel Microbial Factories* — **Zengyi Shao**

**(598) Advances in Optimization with Surrogate and Mixed-Integer Models**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 409

Joseph Scott, Chair  
M. M. Faruque Hasan, Co-Chair

**Sponsored by:** Computers in Operations and Information Processing

**8:00 Paper 598a:** Towards Global Optimization on Low-Dimensional Surrogates Via Manifold Learning — **Felix Dietrich**, Logan R. Matthews, Dmitry Pozharskiy, Ioannis G. Kevrekidis

**8:19 Paper 598b:** On the Derivation of Piecewise Linear Continuous Approximating Functions — **Lingxun Kong**, Christos T. Maravelias

**8:38 Paper 598c:** Surrogate-Based Optimization Framework in Process Systems Engineering — **Atharv Bhosekar**, Lisia S Dias, Zilong Wang, Marianthi Ierapetritou

**8:57 Paper 598d:** Spatial Branch-and-Bound Optimization Using Surrogate Approximations — **Jianyuan Zhai**, Fani Boukouvala

**9:16 Paper 598e:** Reduced Space Formulation for Global Optimization with Artificial Neural Networks Embedded — **Artur M. Schweidtmann**, Alexander Mitsos

**9:35 Paper 598f:** Optimization of Data-Dependent Mixed-Integer Nonlinear Problems — **Sun Hye Kim**, Fani Boukouvala

**9:54 Paper 598g:** On Discretization Based Global Optimization for Mixed-Integer Bilinear Programs — **Xin Cheng**, Xiang Li

**10:13 Paper 598h:** Quadratic Cut Decomposition Method for Convex Mixed-Integer Nonlinear Programs — **David E. Bernal**, Lijie Su, Lixin Tang, Ignacio E. Grossmann

**(599) Alternative Fuels and Enabling Technologies I**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 323

Helen Lou, Chair  
Karthikeyan K. Ramasamy, Co-Chair

**Sponsored by:** Alternate Fuels and New Technology

**8:00 Paper 599a:** Experimental Study of Upper and Lower Flammability Limits of Syngas Mixtures — **Casey C. Fuller**, James Stephen, Seong Kim, Ponnuthurai Gokulakrishnan

**8:17 Paper 599b:** Co-Production of Methanol and Dimethyl Ether Using a Zinc Carbonate Modified Catalyst System — *Lujie Ye, Sunggyu Lee*

**8:34 Paper 599c:** Experimental Investigation of Combustion Characteristics of a Heating Furnace By Hydrogen/Air Micro-Jet Diffusion Flame — *Jun Li, Hongyu Huang, Noriyuki Kobayashi*

**8:51 Paper 599d:** Development of Integrated Geothermal District Heating and Cooling (GDHC) System at West Virginia University Campus-Morgantown, WV — *Nagasree Garapati, Oluwasogo Alonge, Daniel Lemasters, Stephen Vozniak, Lisa Saurborn, Brian Anderson*

**9:08 Paper 599e:** Prevention of Thermal Runaway and Heat Propagation in Battery Module using PCM and Microchannel Plate Cooling System during Nail Penetration — *Young-Gak Yoon, Hye-Ri Gye, Chul-Jin Lee*

**9:25 Paper 599f:** Combustion of an Aqueous Urea/Ammonium Nitrate Alternative Fuel at High Pressure — *Bar Mosevitzky, Michael Epstein, Gennady E. Shter, Gideon S. Grader*

**9:42 Paper 599g:** Stabilizing Phenolic Oil from Pyrolysis of Lignocellulose for Use in Two-Stroke Marine Diesel Engines — *Marjorie R. Rover, Ryan G. Smith, Robert C. Brown*

**9:59 Paper 599h:** Reformulation of Gasoline to Replace Aromatics By Biomass-Derived Oxygenates — *Gourav Shrivastav, Tuhi Suvra Khan, Manish Agarwal, M. Ali Haider*

**10:16 Paper 599i:** H<sub>2</sub> Production Via Ferrite Based H<sub>2</sub>O Splitting Cycle: Solar Reactor Thermodynamic Efficiency Analysis — *Rahul Bhosale, Gorakshnath Takalkar*

**(600) Applications in Immunology and Immunotherapy**  
**Thursday, Nov 1, 8:00 AM**  
Westin Convention Center, Washington

Adriana San-Miguel, Chair  
Jason E. Shoemaker, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**8:00 Paper 600a:** Assessing the Role of Chromatin in Decoding NF- $\kappa$ B Signals — *Shibin Mathew, Victor Wong, Kathryn Miller-Jensen, Suzanne Gaudet*

**8:18 Paper 600b:** Computational Model Predicts the Mechanism of CD28 Co-Stimulation in CAR-Engineered T Cells — *Jennifer A. Rohrs, Elizabeth Siegler, Pin Wang, Stacey D. Finley*

**8:36 Paper 600c:** Heterotypic Interactions with an Endothelial Lumen Increase Neutrophil Lifetime and Migration to *Pseudomonas Aeruginosa* Via IL6 Signaling — *Laurel Hind, Patrick N. Ingram, David J. Beebe, Anna Huttenlocher*

**8:54 Paper 600d:** Using Uncertainty to Assess Feedback Mechanisms in the Innate Immune DNA Sensing Pathway — *Robert W. Gregg, Saumenda N. Sarkar, Jason E. Shoemaker*

**9:12 Paper 600e:** Antigen Discrimination at B Cell Surfaces: Probing the Role of Mechanical Forces — *Bing Li, Steven M. Abel*

**9:30 Paper 600f:** Design of an Optimal Temporal Immunization Strategy for Evolving Broadly Neutralizing Antibodies Against HIV — *Kayla Sprenger, Joy Louveau, Arup Chakraborty*

**9:48 Paper 600g:** Invited Speaker: Engineering Next-Generation T Cells for Cancer Immunotherapy — *Yvonne Y. Chen*

**(601) Big Data in Chemical and Pharmaceutical Processes**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 410

Ravendra Singh, Chair  
Q. Peter He, Co-Chair

**Sponsored by:** Data and Information Systems

**8:00 Paper 601a:** Machine Learning for Automated Meal Detection in Glucose Control Systems for People with Diabetes — *Sediqueh Samadi, Mudassir Rashid, Iman Hajizadeh, Jianyuan Feng, Mert Sevil, Caterina Lazaro, Nicole Hobbs, Rachel Brandt, Ali Cinar*

**8:19 Paper 601b:** Source Analysis of Process Variability in Multi-Step Bio-Process Manufacturing — *Yuan Jin, S. Joe Qin, Victor M. Saucedo, Zheng Li, Angela Meier, Siddhartha Kunda, Briana Lehr, Salim Charaniya*

**8:38 Paper 601c:** Multi-Rate Hard and Soft Sensors Fusion for Monitoring Chemical Processes — *Zhenyu Wang, Leo H. Chiang*

**8:57 Paper 601d:** A New Big Data Benchmark Problem: Fluid Catalytic Cracker Under Model Predictive Control — *Omar S. Santander, Michael Baldea*

**9:16 Paper 601e:** Computation-Driven Mechanistic Understanding of the Cellular Cost and Regulation of Melanin Production — *Rajib Saha, Wheaton Schroeder*

**9:35 Paper 601f:** Using Data Variety for Modeling and Control of Batch Processes — *Abhinav Garg, Prashant Mhaskar*

**9:54 Paper 601g:** Optimal Input and Sensor Selection for System Health Assessment — *Kyle A. Palmer, George M. Bollas*

**10:13 Paper 601h:** Performance Characterization and Fault-Tolerant Control of Multi-Rate Sampled-Data Process Systems with Unknown Measurement Delays — *James Allen, Nael H. El-Farra*

**(602) Biological Conversions and Processes for Renewable Feedstocks**

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 316

Shishir Chundawat, Chair  
Hasan K. Atiyeh, Co-Chair  
Rebecca Ong, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**8:00 Paper 602a:** Comparison of Fructose Production By Sequential vs. Simultaneous Saccharification and Isomerization of CELF Pretreated Corn Stover Solids — *Christian Alcaraz, Rajeev Kumar, Phillip Christopher, Charles E. Wyman*

**8:21 Paper 602b:** Two Different Synthetic Approaches to Obtain Levan Nanoparticles — *Álvaro González-Garcinúño, Celia Nieto, Gema Marcelo, Antonio Tabernero, Miguel A. Galan, Eva Martín del Valle*

**8:42 Paper 602c:** Inhibitory Effect of Hemicellulose Hydrolysates on Glucose Transport across Cell Membrane in Yeast Fermentation — *Xin Tan, Maobing Tu, Changlei Xia*

**9:03 Paper 602d:** Biochar Enhanced Alcohol Production from Syngas By *Clostridium Carboxidivorans* — *Xiao Sun, Hasan K. Atiyeh, Ajay Kumar, Hailin Zhang, Ralph S. Tanner*

**9:24 Paper 602e:** Butanol Production By Fermentation with New Symbiotic Strain TSH06 — *Pengfei Wu, Zhanqian Lin, Shuo Mi, Shuai Mai, Chunkai Gu, Ya Liu, Genyu Wang, Yujie Zhou, Hongjuan Liu, Jianan Zhang*

**(603) Biomaterials for Immunological Applications**

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 331

John Wilson, Co-Chair  
Michael Gower, Co-Chair

**Sponsored by:** Biomaterials

**8:00 Paper 603a:** Immunomodulatory Biomaterials: The Quest for Fundamental Design Rules — *Bret Ulerly*

**8:36 Paper 603b:** Does Co-Encapsulation Matter?: Probing the Biophysical and Functional Impacts of Nanoparticle Combinatorial Delivery — *Patrick Han, Sean Bickerton, Shihan Khan, Jungseok Lee, Eric Song, Omer Mano, Tarek Fahmy*

**8:54 Paper 603c:** Pollen Grains - a Novel Biomaterial for Oral Vaccination — *Md Jasim Uddin, Harvinder Singh Gill*

**9:12 Paper 603d:** Mucosal Polyanhydride Nanovaccine Against Respiratory Syncytial Virus Infection in the Neonatal Calf — *Jodi McGill, Sean Kelly, Pankaj Kumar, Savannah Speckhart, Shannon Haughney, Jamie Henningson, Balaji Narasimhan, Randy Sacco*



Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AICHEvents app.

**9:30 Paper 603e:** Local Induction of Endogenous Regulatory T Cells for the Treatment of Periodontal Disease — **Ashlee Greene**, Mostafa Shehabeldin, Michelle Ratay, Charles Sfeir, Steven R. Little

**9:48 Paper 603f:** Hydrogel-Based Cell Culture System for Scalable Expansion of Human Primary T Cells — **Haishuang Lin**, Qiang Li, Ou Wang, Yuguo Lei

**10:06 Paper 603g:** Transforming Immunotherapy with Nature-Inspired Engineering — **Matthew H. W. Chin**, Marc-Olivier Coppens, Eileen Gentleman, Richard Day

#### (604) Biomimetic Materials

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 328

Vamsi K. Yadavalli, Co-Chair  
Samira M. Azarin, Co-Chair  
Nitin Agrawal, Co-Chair

**Sponsored by:** Biomaterials

**8:00 Paper 604a:** Developing Novel Therapeutic Contact Lenses for the Treatment of Glaucoma Via Macromolecular Memory — **Liana Wuchte**, Amanda Burke, Nicholas Pisani, Mark E. Byrne

**8:18 Paper 604b:** Organic Matrix-Mediated Biomineral Formation and Control — **Gopichand Mallam**, Marina Tsianou

**8:36 Paper 604c:** Engineering an Adhesive and Injectable Cryogel Scaffold — **Devyesh Rana**, Samantha Johnson, Thibault Colombani, Nasim Annabi, Sidi Bencherif

**8:54 Paper 604d:** Silk Protein Self-Assembly As a Pathway Towards Universal Nano-Thin Coatings — **R. Helen Zha**, Tanner D. Fink, Peyman Delparastan, Joschka Bauer, Anika Winkler, Thomas Scheibel, Phillip Messersmith

**9:12 Paper 604e:** Optimizing the Production of a Blue-Absorbing Proteorhodopsin for the Construction of a Multi Wavelength Biological Photodetector — **Jessica Soto-Rodriguez**, Zahra Hemmatian, Marco Rolandi, François Baneyx

**9:30 Paper 604f:** Self-Organization of Molecular Motors in Biopolymer Droplets — **Kimberly L. Weirich**, Kinjal Dasbiswas, Thomas A. Witten, Suriyanarayanan Vaikuntanathan, Margaret L. Gardel

**9:48 Paper 604g:** Correlating Solid-Binding Peptide Structure with Biomimetic Function — **Brittney Hellner**, Kayla Sprenger, Harley Pyles, Arushi Prakash, Jim Pfandner, David Baker, François Baneyx

**10:06 Paper 604h:** Collagen-Based Dispersions and Associated Applications — **Gennaro J. Maffia**, Amanda Peterman

#### (605) Catalysis for C1 Chemistry III: Methane and CO<sub>2</sub>

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 403

Unmesh Menon, Chair  
Marat Orazov, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 605a:** Methane Conversion Using Catalytic Melts to Produce Separable Carbon and Hydrogen or Electrical Power — **David Chester Upham**, Michael Gordon, Horia Metiu, Eric W. McFarland, Zachary Snodgrass

**8:18 Paper 605b:** NiCe@SiO<sub>2</sub> Multi-Yolk-Shell Nanotube Catalyst for Tri-Reforming of Methane — **Sunkyu Kim**, Nicole Cordonnier, Jochen Lauterbach, Erdem Sasmaz

**8:36 Paper 605c:** Dynamics and Mechanism of Carbon Filament Formation during Methane Reforming on Supported Nickel Catalysts — **Samuel L. Leung**, Junmei Wei, William L. Holstein, Miguel Avalos-Borja, Enrique Iglesias

**8:54 Paper 605d:** Fabrication of Fe<sub>2</sub>C Embedded in Hollow Carbon Spheres: A High-Performance and Stable Catalyst for Fischer-Tropsch Synthesis — **Shouying Huang**, Xinbin Ma

**9:12 Paper 605e:** Carbonate-Catalyzed CO<sub>2</sub> Hydrogenation — **Amy Frankhouser**, Aanindeeta Banerjee, Dianne Xiao, Matthew Kanan

**9:30 Paper 605f:** Bifunctional Catalysts for CO<sub>2</sub> Conversion to Plastics, Chemicals and Fuels — **Marc D. Porosoff**

**9:48 Paper 605g:** Support and Promoter Effects on the Activity of Transition Metal Phosphide Catalysts for CO and CO<sub>2</sub> Hydrogenation — **Melis S. Duyar**, Eduardo Valle, Alessandro Gallo, Jonathan Snider, Thomas F. Jaramillo

**10:06 Paper 605h:** Tuning Ni-Catalyzed CO<sub>2</sub> Hydrogenation Pathways Via Ni-Ceria Support Interactions and Ni-Fe Bimetallic Formation — **Lea Winter**, Jingguang G. Chen

**(606) Catalysis with Microporous and Mesoporous Materials III: Fundamental Catalysis and Structure-Property Relations**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 404

Viktor J. Cybulskis, Chair  
Qinghe Zheng, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 606a:** Structure-Function Relationships for Non-Precious Bimetallic MOF-Derived Catalysts in Vapor-Phase Furfural Hydrogenation — **Kristina Golub**, Taylor Sulmonetti, Lalit A. Darunte, Christopher W. Jones

**8:20 Paper 606b:** Cage-Defining Ring: A New Molecular Sieve Structural Indicator for Olefin Product Distribution from the Methanol-to-Olefins Reaction — **Jong Hun Kang**, Stacey I. Zones, Mark E. Davis

**8:40 Paper 606c:** *Ab-Initio* modeling of Site Interconversion and Microkinetic Modeling of Lewis Acid Zeolites for Butadiene Synthesis — **Brandon C. Bukowski**, Jason S. Bates, Rajamani Gounder, Jeffrey Greeley

**9:00 Paper 606d:** Predicting Molecular Adsorption Entropies in Confined Environments — **Paul J. Dauenhauer**, Omar A. Abdelrahman

**9:20 Paper 606e:** The Catalytic Consequences of Silanol Densities within Titanium BEA on Alkene Epoxidation with Hydrogen Peroxide — **Daniel T. Bregante**, Alayna Johnson, Ami Patel, Zeynep Ayla, David W. Flaherty

**9:40 Paper 606f:** Ring-Expansion Carbonylation of Heterocycles By Bimetallic Ion-Pair Catalysis in Co(CO)<sub>4</sub>—Incorporated Cr-MIL-101 — **Hoyoung D. Park**, Mircea Dincă, Yuriy Román-Leshkov

**10:00 Paper 606g:** Zr Metal–Organic Framework As a Catalyst Support for Solid Acid Catalyzed C–C Bond Isomerization and Disproportionation — **Sol Ahn**, Omar K. Farha, Justin M. Notestein

**(607) Cell Biomechanics, Adhesion and Migration II: Cell Movement**  
**Thursday, Nov 1, 8:00 AM**  
Westin Convention Center, Cambria

Amir M. Farnoud, Co-Chair  
Umut Gurkan, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**8:00 Paper 607a:** Feeling the Squeeze: How Motile Cells Respond to Confined Environments — **Emily Wisniewski**, Panagiotis Mistriotis, Robert Law, Kaustav Bera, Soontorn Tuntithavornwat, Nicolas Perez, Alexandros Afthinos, Runchen Zhao, Eda Erdogmus, Catharine Wain, Sean X. Sun, Petr Kalab, Konstantinos Konstantopoulos

**8:18 Paper 607b:** Directional Cell Migration Decision Making in 3D Confinement — **Runchen Zhao**, Alexandros Afthinos, Konstantinos Konstantopoulos

**8:36 Paper 607c:** Fibroblasts Promote Macrophage Migration in 3D Collagen Matrices through Tunnel Formation and Fiber Alignment — **Andrew Ford**, Sophia Orbach, Padmavathy Rajagopalan

**8:54 Paper 607d:** Cadherin 11 Modulate Fibroblast Growth Via Cooperation with Platelet Derived Growth Factor Receptor Beta — **Yayu Liu**, Sindhu Row, Stelios T. Andreadis

**9:12 Paper 607e:** The Role of the Linc Complex in Cell Migration — **Andrew Tamashunas**, David Odde, Richard Dickinson, Tanmay Lele

**9:30 Paper 607f:** Biomechanics Study of Endothelial Cellular Membranes Under Hypo-Osmotic Challenge — **Manuela A.A. Ayee**, Irena Levitan

**9:48 Paper 607g:** Red Blood Cell Adhesion to Heme-Activated Endothelial Cells in Microscale Flow — **Erdem Kucukal**, Anton Ilich, Jane Little, Nigel Key, Umut Gurkan

**10:06 Paper 607h:** The Effect of Rigid Red Blood Cells on Platelet Margination and Adhesion in Flow — **Alison Banka**, Mario Gutierrez, Omolola Eniola-Adefeso



**(608) Charged and Ion-Containing Polymers****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 327

Allie Obermeyer, Chair  
Vivek Sharma, Co-Chair**Sponsored by:** Polymers**8:00 Paper 608a:** Effects of Charge Connectivity, Ion Binding, and Backbone Hydrophilicity on Polyelectrolyte Coacervation — **Jian Qin****8:30 Paper 608b:** Dynamics of Liquid Coacervates Formed By Oppositely Charged Polyelectrolytes — **Christian Aponte-Rivera, Michael Rubinstein****8:45 Paper 608c:** Polyelectrolyte Complexation of Conjugated Polyelectrolytes for Mixed Conductive Complex Fluids — **Scott P.O. Danielsen, Glenn H. Fredrickson, Rachel A. Segalman****9:00 Paper 608d:** A Materials Genome Approach for Enabling Designer Block Polyelectrolytes — **Jeffrey M. Ting, Hao Wu, Abraham Herzog-Arbeitman, Joseph D. Mitchell, Siqi Meng, Matthew V. Tirrell****9:15 Paper 608e:** Phase Behavior and Salt Partitioning in Polyelectrolyte Complexes — **Lu Li, Samanvaya Srivastava, Marat Andreev, Amanda B. Marciel, Jeffrey M. Ting, Juan J. de Pablo, Matthew V. Tirrell****9:30 Paper 608f:** Sequence Control of Complex Coacervation — **Li-Wei Chang, Tyler Lytle, Charles E. Sing, Sarah L. Perry****9:45 Paper 608g:** Ion Transport in Dynamic Poly(Ionic Liquid) Networks Based on Metal-Ligand Coordination — **Gabriel E. Sanoja, Nicole S. Schausser, Joshua M. Bartels, Christopher M Evans, Matthew E. Helgeson, Ram Seshadri, Rachel A. Segalman****10:00 Paper 608h:** The Relationship between Glass Formation and Ion Conductivity in Polymeric Ionic Liquids — **Tarak Patra, David S. Simmons****10:15 Paper 193bd:** Design of Side Chains in P3HT-like Molecules for Maximizing Ionic Conductivity — **Christian Nowak, Mayank Misra, Fernando Escobedo****(609) Charged Polymers for Membrane-Based Water and Energy Applications****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 305

Geoffrey M. Geise, Co-Chair  
William A. Phillip, Co-Chair  
Dongmei Li, Co-Chair**Sponsored by:** Membrane-Based Separations**8:00 Paper 609a:** Anion Exchange Membranes: Towards Extreme Stability and High Conductivity — **Yoonseob Kim, Timothy Swager****8:20 Paper 609b:** Anion Exchange Membranes with Responsive Properties — **Clara Capparelli, Carlos R. Fernandez Pulido, Michael A. Hickner****8:40 Paper 609c:** Nano- and Mesoscale Transport and Mechanics in Ionomers — **Andrew Crothers, Ahmet Kusoglu, Clayton J. Radke, Adam Weber****9:00 Paper 609d:** Elucidating the Effects of Pattern Geometry on Ion Transport through Charge Patterned Membranes — **Feng Gao, William A. Phillip****9:20 Paper 609e:** Ion Diffusion Coefficients in Ion-Exchange Membranes: Significance of Counter-Ion Condensation — **Jovan Kamcev, Gerald S. Manning, Donald R. Paul, Benny D. Freeman****9:40 Paper 609f:** Novel Charge Mosaic Membranes for Desalination — **Gazelle Vaseghi, Ngoc Lien Mai, Glenn Lipscomb****10:00 Paper 609g:** Influencing Transport Properties in Polymerized Ionic Liquids through Ion Chemistry — **Jordan R. Keith, Nathan Rebello, Venkat Ganesan****(610) Crystallization Process Development****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 302

Thomas Vetter, Chair  
Bruce D. Hook, Co-Chair**Sponsored by:** Crystallization and Evaporation**8:00** Introductory Remarks**8:05 Paper 610a:** From Batch to Continuous Reactive Crystallization: A Case Study on Beta-Lactam Antibiotics — **Matthew A. McDonald, Andreas S. Bommarius, Martha A. Grover, Ronald W. Rousseau****8:25 Paper 610b:** A New Slurry Reactive Crystallization to Improve Process Robustness and Scalability — **Lotfi Derdour****8:45 Paper 610c:** Crystallization Process Development of Large Size TMP Crystals — **Qing Lu, Hua Sun, Min Su****9:05 Paper 610d:** Polymorph Selection in Continuous Crystallizers in the Presence of Wet Milling — **Yang Li, Thomas Vetter****9:25 Paper 610e:** Polymorph Dynamics of 2-Aminobenzoic Acid System in Continuous Oscillatory Baffled Crystallizer — **Shivani Kshirsagar, Zoltan K. Nagy****9:45 Paper 610f:** In-Situ Optical Imaging and X-Ray Diffraction Techniques to Probe Organic Molecule Thin Film Crystallization — **Gaurav Giri****10:05 Paper 610g:** Imaging Crystallization Using Deep Learning to Quantitatively Track the Polymorphic Transformation of Carbamazepine — **Zhenguo Gao, Yuanyi Wu, Junbo Gong, Ying Bao, Jingkang Wang, Sohrab Rohani****10:25** Concluding Remarks**(611) Data Mining and Machine Learning in Molecular Sciences II****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 308

Johannes Hachmann, Chair  
Andrew Ferguson, Co-Chair**Sponsored by:** Computational Molecular Science and Engineering Forum**8:00 Paper 611a:** Open Chemistry and Jupyter: Platform for Data Mining and Machine Learning — **Marcus D. Hanwell****8:15 Paper 611b:** Pythia: A Toolbox for Structural Analysis with Machine Learning — **Matthew Spellings, Julia Dshemuchadse, Sharon C. Glotzer****8:30 Paper 611c:** Moleculenet: A Benchmark for Molecular Machine Learning — **Zhenqin Wu, Bharath Ramsundar, Joseph S. Gomes, Evan N. Feinberg, Caleb Geniesse, Aneesh S. Pappu, Karl Leswing, Vijay Pande****8:45 Paper 611d:** Towards an Open-Source Implementation of Spatially-Resolved Molecular Fingerprinting Methods in Machine Learning-Based Predictions of Material Properties — **Mardochee Reveil, Paulette Clancy****9:00 Paper 611e:** Bayesian Optimization of Molecular Structures: Data-Driven Sampling for Molecular Conformers — **Geoffrey Hutchison****9:15 Paper 611f:** End-to-End Learning for Prediction of Optoelectronic Properties of Organic Photovoltaic Polymers — **Peter St. John, Caleb Phillips, Nolan Wilson, Mark R. Nimlos, Travis W Kemper, Ross E Larsen****9:30 Paper 611g:** Practical Applications of Machine Learning to Catalyst Design and Discovery — **Zachary Ulissi****9:45 Paper 611h:** Mapping Configurationally-Dependent Electronic Structure to Coarse-Grained Models with Machine Learning — **Nicholas Jackson, Venkatram Vishwanath, Juan J. de Pablo****10:00 Paper 611i:** Role of Pore Chemistry and Topology in the CO<sub>2</sub> Capture Capabilities of MOFs: Molecular Simulation and Machine Learning — **Ryther Anderson, Jacob Rodgers, Diego Gomez Gualdrón****10:15 Paper 611j:** Accelerating the Characterization and Design of Nanoporous Materials with Data-Driven Models — **Benjamin Bucior, N. Scott Bobbitt, Timur Islamoglu, Subhadip Goswami, Arun Gopalan, Taner Yildirim, Omar K. Farha, Neda Bagheri, Randall Q. Snurr****(612) Diffusion, Transport and Dynamics in Adsorption Systems****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 310

Enzo Mangano, Chair  
Joshua A. Thompson, Co-Chair**Sponsored by:** Adsorption and Ion Exchange**8:00 Paper 612a:** Applying the Wave Theory to Fixed-Bed Dynamics of Metal-Organicframeworks Exhibiting Stepped Adsorption Isotherms: Water/Ethanolseparation on ZIF-8 — **Julien Cousin-Saint-Remi, Jaeri Denayer****8:21 Paper 612b:** Microscopic Diffusion of Mixed and Pure Gases in Mixed Linker ZIF-7-8 — **Samuel Berens, Maitlin Riffele, Febrian Hillman, Hae-Kwon Jeong, Christian Chmelik, Jörg Kärger, Sergey Vasenkov****8:42 Paper 612c:** Process Analysis of Amine-Functionalized Adsorbents for CO<sub>2</sub> Capture Applications — **Lalit A. Darunte, Trisha Sen, Krista S. Walton, David S. Sholl, Matthew J. Realff, Christopher W. Jones**

**9:03 Paper 612d:** Transport of Carbon Dioxide in a Carbon Molecular Sieve — *Stefano Brandani, Enzo Mangano, Federico Brandani, Pluton Pullumbi*

**9:24 Paper 612e:** Gas Sorption, Kinetics of Sorption and Characterization of the Gas Permeation in the Pores of Microporous Metal Organic Frameworks (MOFs) — *Carlos Landaverde-Alvarado, Stephen M. Martin*

**9:45 Paper 612f:** Fast and Highly Selective CO<sub>2</sub> Adsorbent: Li<sup>+</sup>/ZSM-25 Zeolite — *Jianhua Zhao, Ke Xie, Gang Li, Ranjeet Singh, Gongkui Xiao, Qinfen Gu, Penny Xiao, Paul A. Webley*

**10:06 Paper 612g:** Rapid CO<sub>2</sub> Capture from Ambient Air By Electrospun Particle/Fiber Composite Adsorbents — *Bin Mu*

**(613) Distributed Chemical and Energy Processes for Sustainability**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 317

Shweta Singh, Chair  
Carole Read, Co-Chair  
Paul E. Yelvington, Co-Chair

**Sponsored by:** Sustainable Energy

**8:00 Paper 613a:** Photovoltaic/Thermal Energy Addition to Expeditionary Buildings — *Michael Tomac, Shannon Morse, Mike Farrington, David J. Dixon, Braden Baumgardner, Raymond Petty, Joel Bogaert, Reza Salavani*

**8:22 Paper 613b:** An Integrated Approach to Water-Energy Nexus with Multiple Energy Sources — *Fadhil Y. Al-Aboosi, Mahmoud M. El-Halwagi*

**8:44 Paper 613c:** The “Green Latrine”: Deployable Latrine with Off-Grid Photovoltaic/Thermal Energy — *Michael Tomac, Shannon Morse, David J. Dixon, Mike Farrington, Raymond Petty, Joel Bogaert, Braden Baumgardner, Reza Salavani*

**9:06 Paper 613d:** Optimization of Hybrid RO-PRO Membrane Processes at the Water-Energy Nexus — *Mingheng Li*

**9:28 Paper 613e:** An Integrated and Distributed Anaerobic Digestion Waste-to-Energy System for Energy Recovery from Food Waste — *Tong Yen Wah, Jingxin Zhang, Kai Chee Loh*

**9:50 Paper 613f:** Chemical Looping Based Hydrogen Production from Ammonia: System Analysis and Experiments of a Two Reactor and a Three Reactor System — *Mandar Kathe, Deven Baser, Kate Clelland, Andrew Tong, L.-S. Fan*

**10:12 Paper 613g:** Process Intensification of Bio-Ethanol Dehydration Under Compressed Liquid Phase Conditions — *Deanna Poirier, Alex Maag, Geoffrey Tompsett, Michael T. Timko*

**(614) Effects of Confinement on Molecular Properties**

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 307

Liangliang Huang, Chair  
Liquan Zhang, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**8:00 Paper 614a:** Molecular Dynamics Simulation As an Aid for Enhanced Oil and Gas Recovery in Tight and Shale Reservoirs — *Mirella S. Santos, Muhammad Hamza, Luis F.M. Franco, Marcelo Castier, Ioannis G. Economou*

**8:14 Paper 614b:** Complex Behavior of Ordered and Ice-like Water in Carbon Nanotubes Near the Bulk Boiling Point — *José Cobeña, Muhammad Sahimi*

**8:28 Paper 614c:** In-Situ FTIR Study of Effects of Confinement in Mesoporous Silica on Hydration of Ionic Liquids — *Yuxin He, Daudi Saang'onyo, Folami Ladipo, Barbara L. Knutson, Stephen E. Rankin*

**8:42 Paper 614d:** Confinement Effect on Water Transport in CNT Membranes: A Nonequilibrium Molecular Dynamics Study — *Jiabo Tao, Xianyu Song, Teng Zhao, Shuangliang Zhao, Honglai Liu*

**8:56 Paper 614e:** A ‘2D Route’ to the Effective Tangential Pressure in Adsorbed Films: High-Density Equation of State for a Two-Dimensional Lennard-Jones Solid — *Kaihang Shi, Kai Gu, Yifan Shen, Deepti Srivastava, Erik E. Santiso, Keith E. Gubbins*

**9:10 Paper 614f:** Investigation of the Separation of Carbon Dioxide from Methane Using Confined Deep Eutectic Solvents and Ionic Liquids: A Molecular Dynamics Study — *Yan Shen, Francisco R. Hung*

**9:24 Paper 614g:** Ion Diffusion and Capacitance in Electrochemical Systems with Aqueous Electrolytes — *Shuangliang Zhao, Jun Lei, Leying Qing, Honglai Liu*

**9:38 Paper 614h:** Phase Equilibria of Triangle-Well Fluids Confined inside Slit Pores: A Transition Matrix Monte Carlo Simulation Study — *Angan Sengupta, Jhumpa Adhikari*

**9:52 Paper 614i:** The Structure, Dynamics and Relaxation of Water Confined in Graphene Oxide Slit Pores — *Rajasekaran M., K. G. Ayappa*

**10:06 Paper 614j:** Hydrophobic N-doped Biocarbon with High Adsorption Selectivity and Capacity for Benzene Series VOCs under Humid Conditions and Ultralow Pressures — *Meiping Zhu, Xin He, Zhenxia Zhao, Zhangfa Tong*

**10:20 Paper 614k:** PC-SAFT-DFT Development for the Complex Fluids Confined in Pores — *Gulou Shen, Xiaohua Lu, Xiaoyan Ji*

**(615) Emulsions and Foams I**  
**Thursday, Nov 1, 8:00 AM**  
Omni William Penn Hotel, Conference Center A

Xue Chen, Chair  
Peter J. Beltramo, Co-Chair

**Sponsored by:** Interfacial Phenomena

**8:00 Paper 615a:** Effect of Nonfluorinated Surfactants on the Interfacial Stabilization of CO<sub>2</sub>-in-Water (C/W) Emulsion: A Molecular Dynamics Simulation — *Dong-dong Hu*

**8:15 Paper 615b:** The Influence of Nanoparticle Morphology on Surfactant-Nanoparticle Interactions in Emulsions — *Ashwin Kumar Yegya Raman, Clint P. Aichele*

**8:30 Paper 615c:** Surfactant-Induced Nanoparticle Amphiphilicity for Generation and Stabilization of Carbon Dioxide-in-Brine Foams in High Salinity at High Temperature — *Shehab Alzobaidi, Michael Bloom, Congwen Lu, Clark Vu, Nava Rabat-Torki, Andrew J. Worthen, Chola Dandamudi, Caleb Alexander, Will Hardin, Masa Prodanovic, Keith Johnston*

**8:45 Paper 615d:** Suppression of Spontaneous Emulsification with Organic Salts — *Nishat Anjum, Joseph Griesel, Joseph Ritz, Ya-Wen Chang*

**9:00 Paper 615e:** Dynamics of Nucleation in 2D Monodisperse Oil-in-Water Emulsions — *Samira Abedi, Chau-Chyun Chen, Siva A. Vanapalli*

**9:15 Paper 615f:** Interfacial Properties and Spontaneous Emulsification with Block Copolymer Surfactants — *Michael L. Davidson, Moshe Gottlieb, Lynn M. Walker*

**9:30 Paper 615g:** Formation of Multi-Nanoemulsions for Colloidal Synthesis — *Mengwen Zhang, Paula Malo de Molina, Matthew E. Helgeson*

**9:45 Paper 615h:** Shaping Nanoparticle Fingerprints at the Interface of Cholesteric Liquid Crystal Droplets — *Lisa Tran, Hye-Na Kim, Ningwei Li, Shu Yang, Kathleen J. Stebe, Randall D. Kamien, Martin F. Haase*

**10:00 Paper 615i:** Advanced Double Emulsion Templating of Silica Microreactors — *Maritza Mujica, Sven H. Behrens, Victor Breedveld, Michael A. Filler*

**(616) Energetic Materials: Engineered Particles and Interfaces II**

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 412

Edward Dreizin, Chair  
Lori J. Groven, Co-Chair

**Sponsored by:** Energetics

**8:00 Paper 616a:** Mechanoactivation, Initiation and Combustion of Aluminum and Copper Oxide Mixtures — *Aleksandr Dolgoborodov*

**8:15 Paper 616b:** Aluminum-Nickel Fluoride Reactive Materials — *Siva Kumar Valluri, Daniela Bushiri, Mirko Schoenitz, Edward L. Dreizin*

**8:30 Paper 616c:** Combustion of Fuel-Rich Boron – Metal Fluoride Composites — *Siva Kumar Valluri, Mirko Schoenitz, Edward Dreizin*

**8:45 Break**

**9:00 Paper 616d:** Thermal and Biocidal Inactivation of Di-Isopropyl Methylphosphonate and Tributylphosphate through Static and Transient Heating — *Patrick Sanderson, Liyun Feng, James B. Michael, Travis R. Sippel*

**9:15 Paper 616e:** The Characterization of a TNT/Aniline Co-Crystal Solvate: Physicochemical, Explosive Properties and Kinetics of Stability — *Yong Joon Lee, Nadia Sultana, Zachary Fondren, Daniel Unruh, Amitesh Maiti, Brandon L. Weeks*

**9:30 Paper 616f:** Transition Metal Catalysts for Boron Ignition and Combustion — *Kerri-Lee A. Chintersingh, Mirko Schoenitz, Edward L. Dreizin*

**(617) Fluidization in Chemical Looping Processes (Area 20B)****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 415

Fanxing Li, Chair  
Shyam Sundaram, Co-Chair**Sponsored by:** Fluidization and Fluid-Particle Systems**8:00 Paper 617a:** Elutriation Comparison of Particle Separation Systems for Chemical Looping Applications — *Michael Bobek, Steven Rowan, Jingsi Yang, Justin Weber, Ronald W. Brault***8:21 Paper 617b:** Numerical Investigation of Scale-up and in-Bed Heat Exchanger on the Hydrodynamic Characteristics of the Fluidized Bed Combustor of Coal Direct Chemical Looping System — *Dawei Wang, Jianhua Pan, Andrew Tong, Liang-Shih Fan***8:42 Paper 617c:** Chemical Looping Combustion from Biomass Derived Syngas Using a Fluidizable Ni-Co-La-V-Al<sub>2</sub>O<sub>3</sub> Oxygen Carrier: CLC Performance and CPFD Modelling — *Imtiaz Ahmed, Samira Rostom, Hugo de Lasa***9:03 Paper 617d:** Modeling of Circulating Fluidized Bed Reactors for the Selective Oxidation of Alkanes By Chemical Looping — *Luke Neal, Vasudev Pralhad Haribal, Fanxing Li***9:24 Paper 617e:** CFD Modeling of a Dual Fluidized-Bed System Using an Eulerian-Lagrangian Approach — *Hui Liu***9:45 Paper 617f:** CFD-DEM with Uncertainty Quantification (UQ) Compared Against Experiments of Horizontal Jets in a Gas-Solid Fluidized Bed — *Peiyuan Liu, Steven R. Dahl, William Fullmer, Christine M. Hrenya***10:06 Paper 617g:** Validation of the Direct Simulation Monte Carlo (DSMC) Method for Simulating Polydisperse Gas-Solid Flows — *Andrew Hong, Aaron Morris***(618) Fundamentals of Catalysis I: Oxides****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 401

Prashant Deshlahra, Chair  
Michal Bajdich, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**8:00 Paper 618a:** Structure and Activity of Alumina-Supported VO<sub>x</sub>-TiO<sub>2</sub> Catalysts — *Izabela A. Samek, N. Scott Bobbitt, Neil M. Schweitzer, Randall Q. Snurr, Peter C. Stair***8:18 Paper 618b:** Controlled Doping of CeO<sub>2</sub>-ZrO<sub>2</sub> Nanoparticles to Modify Catalytic Activity — *Behnam Safavinia, Yuming Wang, Jarod Larriviere, James A. Dorman, Kerry M. Dooley***8:36 Paper 618c:** Descriptors for Reactivity and Selectivity of Dioxxygen Activation Routes on Metal Oxides — *Stephanie Kwon, Prashant Deshlahra, Enrique Iglesia***8:54 Paper 618d:** Towards the Speciation and Reactivity of Facet-Controlled Vanadium Oxide Catalysts — *Nicholas Jaegers, Lu Zhang, Berlin Sudduth, Eric D. Walter, Mark Engelhard, Libor Kovarik, Mary Hu, Feng Gao, Huamin Wang, Yong Wang, Jian Z. Hu***9:12 Paper 618e:** Selective Hydrodeoxygenation of Furfuryl Alcohol on Doped Metal Oxide Catalysts — *Jiayi Fu, Weiqing Zheng, Jonathan Lym, Konstantinos Alexopoulos, Alexander V. Mironenko, Dionisios G. Vlachos***9:30 Paper 618f:** Understanding the Reactivity of Transition-Metal Oxides for Electrochemical Catalysis — *Michal Bajdich***9:48 Paper 618g:** (001)γ-Fe<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub>/Ag: Good Candidates for the Oxygen Reduction Reactions — *Giulia Righi, Rita Magri***10:06 Paper 618h:** Computational Study of Methane Activation on γ-Al<sub>2</sub>O<sub>3</sub> — *Mudit Dixit, Giannis Mpourmpakis, Mitch Cholewinski***(619) Gene Regulation Engineering: Design Principles and Tool Development****Thursday, Nov 1, 8:00 AM**

Westin Convention Center, Westmoreland West-Central

Anushree Chatterjee, Chair  
Lauren Woodruff, Co-Chair  
Albert Keung, Co-Chair**Sponsored by:** Bioengineering**8:00 Paper 619a:** Development of a Novel RNA-Sensing Spatiotemporal Gene Regulation Program for Eukaryotic Systems — *Victoria M. Hunt***8:18 Paper 619b:** Automated Design of Non-Repetitive Genetic Parts Using Non-Repetitive Parts Calculator and Its Application in Characterizing 4,350 Highly Non-Repetitive *E.coli* Promoters — *Ayaan Hossain, Alexander Reis, Sean Halper, Daniel Cetnar, Howard Salis***8:36 Paper 619c:** CHAOS: A Novel Strategy for Restricting Bacterial Evolution By Inducing Epistatic Interactions — *Peter Otoupal, William Cordell, Madeleine Sitton, Vismaya Bachu, Anushree Chatterjee***8:54 Paper 619d:** Mapping the Operational Landscape of microRNAs in Synthetic Gene Circuits — *Tyler Quarton, Kristina Ehrhardt, James Lee, Yi Li, Leonidas Bleris***9:12 Paper 619e:** Enhancer-Mediated Dynamic Gene Control — *Bomyi Lim, Yuji Yamazaki, Siddhartha Jena, Samuel Keller, Michael Levine***9:30 Paper 619f:** Developing a High Affinity, Dynamic Scaffold Toolkit for Intracellular Spatial Organization of Proteins — *Alexander Mitkas, Wilfred Chen***9:48 Paper 619g:** Improving Phenotypes of *Escherichia coli* at the Post-Transcriptional Level By Engineering Poly(A) Polymerase I — *Yinan Wu, Tongjun Xiang, Mei Li, Chong Zhang, Xin-hui Xing***10:06 Paper 619h:** Predicting Coupled Expression Dynamics in Bacterial Operons — *Daniel Cetnar, Xun Tang, Howard Salis***(620) Going to a Decision Point in Sustainability Analysis****Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 320

Gonzalo Guillén-Gosálbez, Chair  
Nagore Sabio, Co-Chair  
Madhav Ghanta, Co-Chair**Sponsored by:** Sustainability**8:00 Paper 620a:** Assessment of the EU Member Countries Electricity Mix Using DEA and Efmixf — *Patricia Zurano-Cervelló, Carlos Pozo Fernández, Josep Maria Mateo-Sanz, Laureano Jiménez, Gonzalo Guillén-Gosálbez***8:25 Paper 620b:** Assessment of Urban Sustainability: An Exploration Based on Two Metrics for the Chicago Metropolitan Area — *Bayou Demeke, Andres Argoti, Anna Dewey***8:50 Paper 620c:** Dimensionality Reduction in Sustainability Assessment: A Combined Use of Mixed-Integer Programming and Data Envelopment Analysis — *Phantisa Limleamthong, Gonzalo Guillén-Gosálbez***9:15 Paper 620d:** Air Emission Reduction Benefits of Biogas Electricity Generation at Municipal Wastewater Treatment Plants — *Daniel Gingerich, Meagan Mauter***9:40 Paper 620e:** Integrating Market Effects into Sustainable Process Design — Application to Urea Production — *Kyuha Lee, Tapajyoti Ghosh, Bhavik R. Bakshi***10:05 Paper 620f:** Design of Residential Polygeneration Systems Applied to Isolated Communities — *Brenda Cansino-Loeza, José María Ponce-Ortega***(621) Innovations in Process Analytical Technology (PAT) and In Situ Analysis****Thursday, Nov 1, 8:00 AM**

Westin Convention Center, Somerset

Jeffrey A. Nye, Chair  
Aaron Moment, Co-Chair**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum**8:00 Paper 621a:** Integration of Orthogonal PAT Tools to Facilitate API Process Development — *Jeffrey A. Nye, Dimitri Skliar, Greg Beutner***8:21 Paper 621b:** Online LC in Support of Data Rich Experimentation — *Shane T. Grosser, Kerstin Zawatzky, Gabriel C. Graffius***8:42 Paper 621c:** Data Reconciliation in the Quality-By-Design (QbD) Implementation of Pharmaceutical Continuous Tablet Manufacturing — *Qinglin Su, Yasasvi Bommireddy, Marcial Gonzalez, Gintaras V. Reklaitis, Zoltan K. Nagy***9:03 Paper 621d:** Near Infrared Hyperspectral Imaging to Monitor Drug Content and Coating Thickness Uniformity of Oral Disintegrating Films during a Continuous Manufacturing Process — *Nareesh Pavurala, Sonal Mazumder, Scott M. Krull, Nima Yazdanpanah, Xiaoming Xu, Xiaochuan Yang, Cassandra Taylor, Thomas O'Connor, Muhammad Ashraf, Celia N. Cruz***9:24 Paper 621e:** Data-Rich Reaction Profiling of Copper-Catalyzed Methoxylation of an Aryl Halide — *Dan Willard, Jonathan P. McMullen, Kevin Sirk, Gabriel C. Graffius***9:45 Paper 621f:** Parameter Estimation of Reaction Kinetics from Spectroscopic Data - Developments and Applications — *Christina Schenk, Lorenz T. Biegler, Lu Han, Jason Mustakis*



**10:06 Paper 621g:** An Application of Portable Raman Spectroscopy for Rapid and Intact Polymorphism Quantitative Analysis of Multi-Component Pharmaceutical Tablets — **Yufeng Quan, Zhixuan Huang, Lina Jia, Yun Cao, Junbo Gong, Da Chen**

### (622) *In Situ and Operando Spectroscopy*

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 406

Juan J. Bravo-Suarez, Chair  
Taejin Kim, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 622a:** Use of *in-Situ* XAS and TXM Techniques for the Simultaneous Determination of Reaction Kinetics and Structural Evolution of CuO during Sulfidation Reactions. — **Dante Simonetti, Adam Hoffman, Sara Azzam, Kai Zhang, Yahong Xu, Simon R. Bare, Yijin Liu**

**8:20 Paper 622b:** *In-Situ* Spectroscopic Evidence for the Mars-Van Krevelen Mechanism in the Rh Single-Atom Catalyzed CO Oxidation — **Ning Yan**

**8:40 Paper 622c:** *Operando* PM-IRAS+Raman Spectroscopy for Elucidating Poisoning Mechanisms of Pd-Based Hydrogen Separation Membranes in Complex Reaction Mixtures — **Casey O'Brien**

**9:00 Paper 622d:** A Near Ambient Pressure (NAP)-XPS Study on Platinum Nanoparticles Supported on Zr-Based Metal Organic Frameworks (MOFs) — **Reza Vakili, Xiaolei Fan, Alex Walton, Chris Hardacre**

**9:20 Paper 622e:** *Operando* IR Spectroscopy of Electrocatalyst Surfaces for Temperature-Dependent Methane Adsorption and Selective Oxidation — **Shu Hu, Zachary Fishman**

**9:40 Paper 622f:** Application of *in-Situ* x-Ray Absorption Spectroscopy for Next-Generation Batteries — **Mohammad Norouzi Banis, Xia Li, Tom Regier, Yongfeng Hu, Tsun-Kong Sham, Andy (X.) Sun**

**10:00 Paper 622g:** *In Situ/Operando* Reaction Cells: Limitations and Opportunities in the UV-Vis and IR Characterization of Catalysts — **Priya Srinivasan, Juan J. Bravo-Suarez**

### (623) *Interfacial Aspects of Oil/Gas Recovery and Remediation*

**Thursday, Nov 1, 8:00 AM**  
Omni William Penn Hotel, Conference Center B

Joseph R. Samaniuk, Chair  
Xue Chen, Co-Chair

**Sponsored by:** Interfacial Phenomena

**8:00 Paper 623a:** Design of Ecofriendly Surfactant Chemical Herders for Maritime Oil Spill Remediation — **Hao Zhou, Charles Maldarelli, George John**

**8:15 Paper 623b:** Ecofriendly Lignin Nanoparticles for Oil-Spill Remediation — **Jin Gyun Lee, Bhuvnesh Bharti**

**8:30 Paper 623c:** Probing the Effect of Oil Type and Saturation on Foam Flow in Porous Media: Core-Flooding Coupled with Nuclear Magnetic Resonance (NMR) Imaging — **Reza Amirmoshiri, Yongchao Zeng, Zeliang Chen, Rouhi Farajzadeh, Sebastien Vincent-Bonnieu, George J. Hirasaki, Sibani Lisa Biswal**

**8:45 Paper 623d:** Study of Interfacial Aspects of Multiphase Fluid Flow in Three-Dimensional Porous Media Using Differential Phase-Contrast (DPC) X-Ray Imaging — **Maha Yusuf**

**9:00 Paper 623e:** Chemical Compositions in Low Salinity Waterflooding of Carbonate — **Maxim Yutkin, Clayton J. Radke**

**9:15 Paper 623f:** Interfacial Tension and Phase Behavior of Pre-Equilibrated Mixtures of Aqueous Solutions of an Isopropoxylated Surfactant and Crude Oil — **Jaeyub Chung, Bryan W. Boudouris, Elias I. Franses**

**9:30 Paper 623g:** The Effect of Pressure on Equilibrium Surfactant Thermodynamics — **Zachary R. Hinton, Nicolas J. Alvarez**

**9:45 Paper 623h:** Stepwise Thinning and Nanoscopic Thickness Variations in Foam Films Formed By Aqueous Sodium Naphthenate Solutions — **Chrystian Ochoa, William Yang, Yiran Zhang, Subinuer Yilixiati, Samanvaya Srivastava, Vivek Sharma**

**10:00 Paper 623i:** Conformable Molecularly Thin Pouches to Hold Oil Droplets in Solution — **Marzhana Omarova, Vijay T. John**

### (624) *Liquid Phase Reaction Engineering*

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 405

Daniel Chen, Chair  
Xinrui Yu, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 624a:** A Computational Fluid Dynamics Study on Reactor Selection for DNA Origami Folding Kinetics — **Tianyi Hua, Ryan L. Hartman**

**8:22 Paper 624b:** Rational Design of Mixed Solvent Environments for Acid-Catalyzed Biomass Conversion Reactions: A Combined Approach Using Experiments and Molecular Simulations — **Theodore Walker, Alex Chew, Huixiang Li, Benginur Demir, Z. Conrad Zhang, George W. Huber, Reid C. Van Lehn, James Dumesic**

**8:44 Paper 624c:** *Reactions and Chemical Kinetics of Amino Acids in Hot Compressed Water* — **James D. Sheehan, Phillip E. Savage**

**9:06 Paper 624d:** Functionalization of Cellulose Surfaces Using Dye Anchors and Click Chemistry — **Christy Wheeler West, Amanda Brown, Charles Moran, Mack Bozman, T. Grant Glover, Kevin N. West**

**9:28 Paper 624e:** Synthesis of Egg-Shell AuPd@SiO<sub>2</sub> Catalysts for Liquid Phase Hydrogenation Reaction of Chloronitrobenzenes to Chloanioline — **Yu-Wen Chen**

### (625) *Lithium and Beyond: Fundamental Advances in High Performance Batteries I*

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 306

Nian Liu, Chair  
Robert J. Messinger, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

**8:00 Paper 625a:** Deconvolution of the Solid-Electrolyte Interphase Growth Patterns on Conversion-Based Transition Metal Oxides — **Benjamin Ng, Alessandro Palmieri, William E. Mustain**

**8:20 Paper 625b:** Determining Passivation Mechanisms in the Solid-Electrolyte-Interphase with Functionalized Molecular Probes and Electrochemical Collector-Generator Measurements — **Oliver Harris, Maureen H. Tang**

**8:40 Paper 625c:** Advanced Li Metal Anode in Safe Rechargeable Batteries — **Xin-Bing Cheng, Xiang Chen, Rui Zhang, Chen-Zi Zhao, Xue-Qiang Zhang, Qiang Zhang**

**9:00 Break**

**9:10 Paper 625d:** Designing Optimal Electrolytes for Next Generation Energy Storage — **Nav Nidhi Rajput, Kristin Persson**

**9:30 Paper 625e:** Modeling of High Transference Number Electrolytes for Fast Charging Lithium Ion Batteries — **Eric McShane, Bryan D. McCloskey**

**9:50 Paper 625f:** Enhancing the Stability of High-Voltage Lithium-Ion Battery By Sulfur-Containing Electrolyte Additives — **Xiaoying Yu, Chao Shang, Qi Wang**

**10:10 Paper 625g:** Long Lasting Li-S Batteries Via Suppressing Lithium Dendrites — **Vilas G. Pol, Patrick Kim, Kyungho Kim**

### (626) *Mechanistic Models for Integrated Pharmaceutical Product and Process Design*

**Thursday, Nov 1, 8:00 AM**  
Westin Convention Center, Fayette

Salvador García-Muñoz, Chair  
Dimitrios I. Gerogiorgis, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**8:00 Paper 626b:** Optimal Design of Separation Systems for Continuous Manufacturing of Nevirapine, an Active Pharmaceutical Ingredient (API) for H.I.V. Treatment — **Samir Diab, Tyler McQuade, Dimitrios I. Gerogiorgis**

**8:30 Paper 626c:** Utilizing Mechanistic Modelling to Assist in the Process Development of Pharmaceutical Drug Substance Processes — **Rosario Porrazzo, Sam Wilkinson, Niall Mitchell**

**9:00 Paper 626d:** System-Model Development for Continuous Drug Substance Manufacturing Process — **Boung Wook Lee, Kehua Yin, Alexander O'Brien, Yangmu C. Liu, Eric Ricci, Brian Roesch, Kevin Splaine**

**9:30 Paper 626e:** An Industrial Application of Parameter Estimation of Biocatalytic Transaminase Reactions — **Javier Magano, David Damon, John Wong, Steven M. Guinness, Ke Wang, Jason Mustakis, Lu Han**

**10:00 Paper 626f:** Investigating the Impact of Water on the Energetics and Kinetics of a Reductive Amination Reaction – a Computational and Experimental Approach — **Aikaterini Diamanti, Carla Luciani, Jonas Y. Buser, Amparo Galindo, Claire S. Adjiman**

#### (627) Membrane Modeling and Simulation

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 304

Nils Tilton, Co-Chair  
Xianghong Qian, Co-Chair  
Martin Maldovan, Co-Chair

**Sponsored by:** Membrane-Based Separations

**8:00 Paper 627a:** Molecular Simulation Insights on Xe/Kr Separation in a Set of Nanoporous Crystalline Membranes — **Ryther Anderson, Ting Wu, Moises Carreon, Diego Gomez Gualdrón**

**8:15 Paper 627b:** The Effect of the Pore Entrance on Particle Motion in Slit Pores: Implications for Ultrathin Membranes — **Ruth E. Baltus, Armin Delavari**

**8:30 Paper 627c:** Non-Equilibrium Molecular Dynamics Simulations of Composite MOF/Polymer Membranes — **Aydin Ozcan, Rocío Semino, Guillaume Maurin, Ozgur Yazaydin**

**8:45 Paper 376ak:** Module-Scale Simulation of Hollow Fiber Vacuum Membrane Distillation Using Openfoam — **Albert Kim, Ho Ji, Siu Fung Tang, Deok-Soo Moon, Hyeon-Ju Kim**

**9:00 Paper 627e:** Understanding Polyether Sulfone Membrane Formation Via Nonsolvent Induced Phase Separation By Dissipative Particle Dynamics (DPD) Simulations — **Yuanhui Tang, David Ford, Xianghong Qian, Paul Millett, M. Rosario Cervellere**

**9:15 Paper 627f:** Computationally Investigating Zeolite Nanosheets As Pervaporation Membranes for Ethanol Extraction and the Role of Membrane Surfaces — **Changlong Zou, Li-Chiang Lin**

**9:30 Paper 627g:** A New Design Strategy for Membrane Gas Separation: Engineered Anisotropic Mass Diffusion — **Juan Manuel Restrepo-Florez, Martin Maldovan**

**(628) Membranes for CO<sub>2</sub> Capture**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 303

W.S. Winston Ho, Co-Chair  
Haiping Lin, Co-Chair  
Alexander Lopez, Co-Chair

**Sponsored by:** Membrane-Based Separations

**8:00 Paper 628a:** Amine-Functionalized Graphene Oxide Hollow Fiber Membranes for CO<sub>2</sub> Capture — **Fanglei Zhou, Huynh Ngoc Tien, Qiaobei Dong, Weiwei Xu, Huazheng Li, Miao Yu**

**8:21 Paper 628b:** High CO<sub>2</sub> Separation Performance of Hydroxide-Ceramic Dual-Phase Membrane — **Azadeh Amiri, Li Sze Lai, Maira R. Ceron, Matthew Merrill, Patrick Campbell, Sangil Kim**

**8:42 Paper 628c:** Atomistic Investigation of CO<sub>2</sub>-Induced Plasticization in PIM-1 Polymer — **Marcel Balçık, M. Goktug Ahunbay**

**9:03 Paper 628d:** Novel Facilitated Transport Membrane for Post-Combustion Carbon Capture: From Membrane Synthesis to Process Design — **Yang Han, W.S. Winston Ho**

**9:24 Paper 628e:** Fabrication and Optimization of SAPO-34 Membranes for Efficient Separation of CO<sub>2</sub>/CH<sub>4</sub> Gas Mixture — **Xiufeng Liu, Baoquan Zhang**

**9:45 Paper 628f:** Ionic Liquids Based Composite Membranes for CO<sub>2</sub> Separation — **Lu Bai, Chenrui Zhang, Bingbing Yang, Jiuli Han, Xiangping Zhang**

**10:06 Paper 628g:** Automated Process Design and Techno-Economic Assessment of Membrane-Based CO<sub>2</sub> Capture Systems — **Jin-Kuk Kim, Seokwon Yun, Sunghoon Lee, Mun-Gi Jang**

#### (629) Modeling, Control, and Optimization of Manufacturing Systems

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 408

Michael Baldea, Chair  
Q. Peter He, Co-Chair

**Sponsored by:** Systems and Process Control

**8:00 Paper 629a:** Real Time Constrained Model Predictive Control for the Continuous Manufacturing of Pharmaceuticals — **Kelly Nocon, Omar Sheikh, Niraj Mehta, Vasilios Manousiouthakis**

**8:19 Paper 629b:** Model Predictive Control of a Rotational Molding Process — **Abhinav Garg, Felipe P.C. Gomes, Prashant Mhaskar, Michael R. Thompson**

**8:38 Paper 629c:** A Multiparametric Programming Based Approach to Integrate Design, Scheduling, and Control of a Batch Process — **Baris Burnak, Efstratios N. Pistikopoulos**

**8:57 Paper 629d:** Multi-Objective Dynamic Optimisation of a Fed-Batch Nosiheptide Reactor — **Alistair D. Rodman, Dimitrios I. Gerogiorgis**

**9:16 Paper 629e:** Big Data and the Chemical Industry: From Sensor to Value — **Flor Castillo, William Hollar**

**9:35 Paper 629f:** Big Data and IoT: A Demonstration Testbed of Multi-Stage Centrifugal Pumping System — **Devarshi Shah, Jin Wang, Q. Peter He**

**9:54 Paper 629g:** Pressure Swing Adsorption Cycle Synthesis Utilizing Artificial Neural Networks As Surrogate Models — **Karson Leperi, Daison Yancy-Caballero, Randall Q. Snurr, Fengqi You**

**10:13 Paper 629h:** Continuous Control of a Polymerization System with Deep Reinforcement Learning — **Yan Ma, Wenbo Zhu, Michael G. Benton, Jose A. Romagnoli**

#### (630) Novel Nanoparticles and Nanostructured Materials for Energy Applications

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 413

Yangchuan Xing, Chair  
Satish K. Nune, Co-Chair  
Alan W. Weimer, Co-Chair

**Sponsored by:** Nanoparticles

**8:00 Paper 630a:** Engineered Electrodes for Energy Storage and Battery Safety — **Vilas G. Pol**

**8:30 Paper 630b:** Extended Surface Electrocatalyst Development Via Atomic Layer Deposition — **William McNeary IV, Audrey Linico, Chilan Ngo, Sarah Zaccarine, Jason Zack, Katherine Hurst, Shaun M. Alia, Scott A. Mauger, K.C. Neyerlin, Karen J. Buechler, Will Medlin, Svitlana Pylypenko, Bryan S. Pivovar, Alan W. Weimer**

**8:55 Paper 630c:** Thin Oxide Film Coatings for Improved Lithium Ion Battery Cathodes — **Amanda Hoskins, Samantha L. Millican, Yan Gao, Xinhua Liang, Alan W. Weimer**

**9:20 Paper 630d:** The Application of Magnesiothermic Reduction of Silica to Produce Porous Silicon for Lithium Ion Batteries — **Jake Entwistle, Siddharth V. Patwardhan**

**9:45 Paper 630e:** Fluidized-Bed CVD of Si@SiC@C-like Nanoparticle and Its Application As Anode Materials — **Chunhui Yu, Chenxi Zhang, Zhexi Xiao, Fei Wei**

**10:10 Paper 630f:** Functional Nanomaterials for OIL and Gas Discovery and Recovery Applications — **Amr Abdel-Fattah, Afran Mashat, Hassan Alqahtani, Nouf Aljabri, Howard Schmidt**

#### (631) Particle Separations (Solid/Solid, Solid/Liquid, Solid/Gas)

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 414

Richard M. Lueptow, Chair  
Hadjira Iddir, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**8:00 Paper 631a:** CFD Modeling of a Dry Electrostatic Protein Separation Approach — **Aram Parsa, Solmaz Tabatabaei, Amin R. Rajabzadeh**

**8:18 Paper 631b:** Measurement of Dewatering Indices to Rank the Ability for a Given Material to Dewater Effectively in a Prescribed Piece of Process Equipment — **Kerry Johanson**

**8:36 Paper 631c:** Separation Performance of a Coupled Cyclone with Built-in Circulating Granular Bed Filter(C-CGBF) — **Sihong Gao, Dandan Zhang, Yiping Fan, Chunxi Lu**

**8:54 Paper 631d:** Numerical Simulation of the Capture of Particles By Dead-End Pores — **Siying Zhang, Joseph J. McCarthy**

#### (632) Polymers in Batteries

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 326

Ying Diao, Chair  
Siamak Nejati, Co-Chair

**Sponsored by:** Polymers

**8:00 Paper 632a:** Electrochemical Kinetics in Solid Electrolytes for Lithium Metal Batteries — **Daniel Hallinan Jr., Marc Berliner, Brandon McGill, Alexander Rausch**

**8:15 Paper 632b:** Ultrathin Polymer Coatings As Artificial Solid Electrolyte Interphases for Lithium Ion Battery Anodes — **Wyatt Tenhaeff, Shaofei Wang, Yifan Gao, Brian Shen**

**8:30 Paper 632c:** Crosslinked Ionomers for Use As Magnesium-Sulfur Battery Cathode Coatings — [Hunter Ford](#), [Laura Merrill](#), [Peng He](#), [Jennifer Schaefer](#)

**8:45 Paper 632d:** Solid Polymer Electrolyte Networks Via the Active Monomer Mechanism for Lithium Ion Conduction — [Ian Hosein](#), [Francielli Genier](#)

**9:00 Paper 632e:** Engineering Ion Transport in Microporous Polymer Separators for Li-S Batteries — [Jonathan E. Bachman](#), [Yi Cui](#)

**9:15 Paper 632f:** Developing Adhesive Coatings to Protect the Lithium Metal Anode — [Chibueze Amanchukwu](#), [Zhenan Bao](#)

**9:30 Paper 632g:** Tuning Semi-Conducting Polymers for Binder Applications in Fe<sub>3</sub>O<sub>4</sub> Li-Ion Battery Anodes — [Krysten Minnici](#), [Yo Han Kwon](#), [Matthew M. Huie](#), [James Ponder](#), [John Reynolds](#), [Kenneth J. Takeuchi](#), [Esther S. Takeuchi](#), [Amy C. Marschillok](#), [Elsa Reichmanis](#)

**9:45 Paper 632h:** Lithium Ion Conducting Multiblock Polymers As Solid-State Electrolytes for Lithium Ion Batteries — [Tzu-Ling Chen](#), [Rui Sun](#), [Carl L. Willis](#), [Brian Morgan](#), [Frederick L. Beyer](#), [Yossef A. Elabd](#)

**10:00 Break**

**10:15 Paper 632j:** Towards Solid Calcium Ion Batteries: Solid and Gel Polymer Electrolytes for Effective Calcium Ion Conduction and Battery Separator Operation — [Ian Hosein](#), [Saeed Biria](#), [Francielli Genier](#), [Jiayue Wang](#), [Shreyas Pathreker](#)

**(633) Rare Earth Elements: Extraction, Separation, Characterization, Economics, Criticality, and Kinetics**

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 321

[Evan J. Granite](#), Chair

**Sponsored by:** Advances in Fossil Energy R&D

**8:00 Paper 633a:** Recovering Rare Earth Elements from Coal-Based Materials — [Mary Anne Alvin](#)

**8:17 Paper 633b:** Transmission Electron Microscopy Observations of Rare Earth Minerals in the Fire Clay Coal, Kentucky, and in the Derived Combustion Ashes — [James C. Hower](#)

**8:34 Paper 633c:** Selectivity and Recovery of Rare Earth Elements from Coal Ash Leachates Using Liquid Membrane-Based Separations — [Ryan Smith](#), [Ross Taggart](#), [Mark R. Wiesner](#), [Heileen Hsu-Kim](#)

**8:51 Paper 633d:** Effect of Calcium Halide Salt Addition on the Fate of Rare Earth Compounds during Coal Combustion Process — [Ward Burgess](#), [Murphy J. Keller](#), [Elliot Roth](#), [Bret H. Howard](#), [Jonathan W. Lekse](#), [Evan J. Granite](#)

**9:08 Paper 633e:** Examination of the Distribution and Form of the Rare Earth Elements in a Metalliferous Lignite Coal — [Brittany Rew](#), [Dan Laudal](#), [Steve Benson](#), [Nolan Theaker](#)

**9:25 Paper 633f:** Economic Extraction, Recovery and Upgrading of Rare Earth Elements from Coal-Based Resources — [Michael Free](#)

**9:42 Paper 633g:** Hydrometallurgical Circuits for the Recovery of RARE Earth Elements from Coal Sources — [Rick Honaker](#)

**9:59 Paper 633h:** Determination and Recovery of Rare Earths from Coal Combustion By-Products — [Evan J. Granite](#), [Ken Ladwig](#), [Elliot Roth](#)

**10:16 Paper 633i:** Evaluation of Critical Trace Elements Including Rare Earth Elements in U.S. Coals — [Ronghong Lin](#), [Yee Soong](#), [Evan J. Granite](#)

**(634) Rational and Computational Techniques for Protein Engineering**

**Thursday, Nov 1, 8:00 AM**  
Westin Convention Center, Butler

[Seok Hoon Hong](#), Chair  
[Tim Whitehead](#), Co-Chair

**Sponsored by:** Bioengineering

**8:00 Paper 634a:** Rational Design of Glucose-Responsive Insulin Using Pharmacokinetic Modeling — [Naveed Bakh](#), [Gili Bisker](#), [Michael A. Lee](#), [Xun Gong](#), [Abel B. Cortinas](#), [Robert Langer](#), [Daniel A. Anderson](#), [Zhen Gu](#), [Sanjoy Dutta](#), [Michael Weiss](#), [Michael Strano](#)

**8:18 Paper 634b:** Computational Design of High-Resolution Protein Crystals — [Jeliazko R. Jeliazkov](#), [Aaron Robinson](#), [James M. Berger](#), [Bertrand E. Garcia-Moreno](#), [Jeffrey J. Gray](#)

**8:36 Paper 634c:** A Novel Approach for the Computational *De Novo* Design of Antibody Structures and Alternative Scaffolds — [Varun Chauhan](#), [Robert Pantazes](#)

**8:54 Paper 634d:** Crystal Structure Based Rational Engineering of Tyrosine Decarboxylase for Efficient Preparation of Tyramine — [Guochao Xu](#)

**9:12 Paper 634e:** Engineering the Active Site Microenvironment of a Thermostable Alcohol Dehydrogenase As a Means to Modulate Kinetic Activity — [Wala Abdallah](#), [Louis Lancaster](#), [Ian Wheeldon](#), [Scott Banta](#)

**9:30 Paper 634f:** Transition Path Methods for Understanding Catalysis By Proteins — [Natasha Seelam](#), [Bruce Tidor](#)

**9:48 Paper 634g:** Invited Speaker - TBA — [Eric Althoff](#)

**(635) Recalcitrance of Woody Biomass**

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 324

[Yaseen Elkasabi](#), Chair  
[Maobing Tu](#), Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**8:00 Paper 635a:** Does Recrystallization in Aqueous Environment Affect the Reactivity of Ball-Milled Cellulose for Acid Catalyzed Hydrolysis? — [Maksim Tyufekchiev](#), [Alex Kolodziejczak](#), [Patricia Guerra](#), [James Meyer](#), [Pu Duan](#), [Frederick Greenaway](#), [Marcus Foston](#), [Klaus Schmidt-Rohr](#), [Michael T. Timko](#)

**8:25 Paper 635b:** Solvent and Processing Conditions for Pretreatment and Dissolution of Cotton Cellulose — [Mohammad Ghasemi](#), [Luz V. Vargas-Aponte](#), [Paschalis Alexandridis](#), [Marina Tsiannou](#)

**8:50 Paper 635c:** Synthesis of Artificial Lignin Polymers and Their Effects on Enzymatic Hydrolysis of Cellulose — [Conghui Yue](#), [Hairong Guan](#), [Maobing Tu](#)

**(636) Self-Assembled Biomaterials**  
**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 311

[Anju Gupta](#), Chair  
[Pooya Davoodi](#), Co-Chair

**Sponsored by:** Bionanotechnology

**8:00 Paper 636a:** Invited Speaker: Polypeptoid Amphiphiles Serve As a Connective Glue to Build Lipid Layers on Vesicles: Fundamentals and Applications to Drug Delivery — [Vijay T. John](#), [Marzhana Omarova](#), [Yueheng Zhang](#), [Donghui Zhang](#)

**8:30 Paper 636b:** Tunable Supramolecular Assembly of Nucleoside Phosphoramidate Nanofibres By Enzyme Activation — [Harrison T. West](#), [Carston R. Wagner](#), [Clifford M. Csizmar](#)

**8:45 Paper 636c:** Programming Hierarchical Supramolecular Architecture in Biomaterials — [Ronit Freeman](#)

**9:00 Paper 636i:** Synergistic Assembly of Peptide Amphiphiles for Encapsulation of Camptothecin — [Steffie Mano](#), [Tong Yen Wah](#)

**9:15 Paper 636e:** Structural Evaluation of Designer Co-Assembling Peptide Nanofibers — [Kong M. Wong](#), [Qing Shao](#), [Dillon T. Seroski](#), [Gregory A. Hudalla](#), [Carol K. Hall](#), [Anant K. Paravastu](#)

**9:30 Paper 636f:** Evidence for Self-Assembly-Driven *Trans*-to-*Cis* Amide Bond Isomerization in Peptoid Nanosheets — [Benjamin C. Hudson](#), [Alessia Battigelli](#), [Michael Connolly](#), [John Edison](#), [Ryan Spencer](#), [Steve Whitlam](#), [Ronald N. Zuckermann](#), [Anant K. Paravastu](#)

**9:45 Paper 636g:** Self Assembly of Silk Fibroin/Metal Composite Nanomaterials — [Alexander Mitropoulos](#), [Gabriella Milanese](#), [Jenny Wang](#), [F. John Burpo](#), [Kamil Woronowicz](#), [Enoch Nagelli](#)

**10:00 Paper 636h:** Redox Sensitive Protein Droplets from Recombinant Oleosin — [Ellen H. Reed](#), [Daniel A. Hammer](#)

**10:15 Paper 636d:** A Way for Controlling Levan Nanoparticles Production Andparticle Size Distribution — [Álvaro González-Garcinúño](#), [Antonio Tabernero](#), [Gema Marcelo](#), [Miguel A. Galán](#), [Eva Martín del Valle](#)

**(637) Semiconducting Quantum Dots and Nanocrystals**

**Thursday, Nov 1, 8:00 AM**  
David L. Lawrence Convention Center, 330

[Ayaskanta Sahu](#), Chair  
[Matthew G. Panthani](#), Co-Chair  
[Ajay Singh](#), Co-Chair

**Sponsored by:** Electronics and Photonics

**8:00 Paper 637a:** Invited: Insulator-Metal Transition in Plasma-Synthesized ZnO Nanocrystal Networks — [Eray S. Aydil](#), [Ben Greenberg](#), [Zachary Robinson](#), [Jacob Held](#), [K. Andre Mkhoyan](#), [Uwe R. Kortshagen](#)



**8:25 Paper 637b:** Active Plasmonics Based Devices Using Metal Oxide Nanocrystals: Fundamental and Applications — **Ankit Agrawal, Delia J. Milliron**

**8:40 Paper 637c:** Metal Oxide Infilling of Quantum Dot Thin Films: Increased Stability and Carrier Mobility for Device Applications — **Fatemeh S. M. Hashemi, Ryan W. Crisp, Jordi Alkemade, Arjan J. Houtepen, J. Ruud van Ommen**

**8:55 Paper 637d:** Understanding Low-Voltage Electrophoretic Deposition of Non-Oxide Semiconductor Nanocrystals — **Aaron T. Fafarman**

**9:10 Break**

**9:20 Paper 637e:** *Invited:* Perovskite Nanocrystals: From Self-Assembly to Exciton Dynamics — **Rizia Bardhan**

**9:45 Paper 637f:** Structural and Compositional Engineering of Visible and Near-Infrared Optical Resonances in Ternary Metal Chalcogenide Nanocrystals — **Soohyung Lee, Vincent C. Holmberg**

**10:00 Paper 637g:** Strained Low Dimensional  $\text{Sr}_{1-x}\text{Ti}_x\text{Nb}_{1-y}\text{O}_{3+\delta}$  nanoparticles for Infrared Light Harvesting — **Tochukwu Ofoegbuna, Pragathi Darapaneni, James A. Dorman**

**10:15 Paper 637h:** Flow Reactors for Quantum Dot Synthesis: Single Nanocrystal Spectroscopy in Flow — **Ioannis Lignos, Hendrik Utzat, Yiming Mo, Mouni G. Bawendi, Klavs F. Jensen**

#### (638) Syngas Production and Gas-to-Liquids Technology

**Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 402

Erdem Sasmaz, Chair  
Hema Ramsurn, Co-Chair  
Amrit Jalan, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 638a:** Production of Jet Fuel from Coal-Derived Syngas — **Santosh Gangwal, Venkat Venkataraman**

**8:20 Paper 638b:** Energy Efficient Methane Reforming Enabled By Continuous Manufacturing of Porous Titania Microparticles — **Zachary Campbell, Matthew Parker, Jacob Lustik, Daniel Jackson, Seif Yusuf, Fanxing Li, Milad Abolhasani**

**8:40 Paper 638c:** Enhanced Methane Conversion in Chemical Looping Partial Oxidation to Syngas Using Copper, Cobalt and Nickel Doping Modification with Density Functional Theory Calculation — **Mengqing Guo, Lang Qin, Zhuo Cheng, Yan Liu, Liang-Shih Fan**

**9:00 Paper 638d:** Modified Ceria for Low-Temperature Methane Partial Oxidation and Water-Splitting — **Vasudev Pralhad Haribal, Courtney Paulus, Arya Shafieifarhood, Fanxing Li**

**9:20 Paper 638e:** Particle-Resolved Simulation of Fixed-Bed Reactors Filled with Complex Particle Shapes — a Validation Study — **Nico Jurtz, Tobias Henkel, Urvashi Srivastava, Matthias Kraume**

**9:40 Paper 638f:** Dry Reforming of Methane over a Ni-Mo Nanocatalyst — **Youngdong Song, Ercan Ozdemir, Aldair Adishev, Saravanan Subramanian, Aadesh X. Harale, Bandar Fadhel, Aqil Jamal, Dohyung Moon, Cafer T. Yavuz**

**10:00 Paper 638g:** Fischer-Tropsch Synthesis over Alumina Supported Cobalt Catalyst in a Fixed-Bed Reactor — **Aaditya Hari Bharanidharan, Mohammed Muzwar, Pushkala Venkatesh, Suresh A.K., Udaya Bhaskar Reddy Ragula**

#### (639) Synthesis and Application of Inorganic Materials: Application

**Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 329

Praveen K. Thallapally, Chair  
Mark A. Snyder, Co-Chair

**Sponsored by:** Inorganic Materials

**8:00 Paper 639a:** Egg-Structural  $\text{Si@Si}_3\text{N}_4\text{@C}$  Anode with Admirable Cyclability, Rate Capability and Initial Coulombic Efficiency — **Zhexi Xiao, Chenxi Zhang, Chunhui Yu, Fei Wei**

**8:19 Paper 639b:** Optimizing Hierarchical Zeolites for Applications in Catalysis — **Maryam Khaleel, Rami Hamaidi, Issam Ismail, Saeed Alhassan**

**8:38 Paper 639c:** Facile Induction of Mesoporosity within Crystalline Metal-Oxides By Hydrogen Peroxide Treatment — **Jonathan Colon, Dmitriy Ruckodanov, John M. Landers, Alexander Neimark**

**8:57 Paper 639d:** Theoretical Investigation of the Electronic, Optical and Thermodynamic Properties of  $\text{La}_x\text{Sr}_{1-x}\text{Co}_y\text{Fe}_{1-y}\text{O}_{3-\delta}$  ( $x, y = 0.0 \sim 1.0$ ) Perovskites — **Ting Jia, Hua Hao, Paul R. Ohodnicki, Benjamin T. Chorpene, Gregory Hackett, Zhi Zeng, Yuhua Duan**

**9:16 Paper 639e:** Amine-Functionalized Graphene Oxide Applied to Temperature-Programmed Carbon Dioxide Adsorption and Desorption — **Nathaniel Dugos, Fritzie Hannah Baldovino, Susan Rocas, Armando Quitain, Tetsuya Kida**

**9:35 Paper 639f:** Colorimetric Sensing and Photocatalytic Decomposition of Mustard Gas Surrogates on Polyoxometalate-Based Oxidants — **Dimitrios A. Giannakoudakis, Jonathan Colon, John M. Landers, Shiva Murali, Marc Florent, Alexander Neimark, Teresa J. Bandosz**

**9:54 Paper 639g:** Construction of Heterojunction in  $\text{In}_2\text{S}_3/\text{NH}_2\text{-MIL-68(In)}$  for Efficient Visible-Light-Induced Hydrogen Production — **Yunhong Pi, Xiye Li, Jing Xiao, Zhong Li**

**10:13 Paper 639h:** Development of Vertically Aligned Boron-Nitride-Nanopore Membranes for Giant Osmotic Power Generation — **Aaditya Pendse, Semih Cetindag, Sanjay Behura, Vikas Berry, Jerry Shan, Sangil Kim**

#### (640) Thermochemical Conversion of Biomass

**Thursday, Nov 1, 8:00 AM**

David L. Lawrence Convention Center, 325

Sudhagar Mani, Chair  
Joseph F. Stanzione III, Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**8:00 Paper 640a:** Effects of Warm Water Washing on the Fast Pyrolysis of *Arundo Donax* — **Devin Chandler, Fernando Resende**

**8:20 Paper 640b:** Ex-Situ Catalytic Cracking of Biomass Pyrolysis Vapors over Montmorillonite K10-Supported Iron (III) Oxide — **Candice Ellison, Dorin Boldor**

**8:40 Paper 640c:** Iron-Based Chemical Looping Biomass Gasification for Carbon Nanofiber Production: Process Simulation and Experiments — **Fanhe Kong, Elliot Kennel, Robert Statnick, Mandar Kathe, Andrew Tong, Chenghao Wang, Dikai Xu, Eric Falascino, Yan Liu, Liang-Shih Fan**

**9:00 Paper 640d:** Techno-Economic Analysis of Simultaneous Biomass Gasification and Syngas Upgrading Via Chemical Looping Technology — **Micah Jasper, Abloghasem Shahbazi, Keith Schimmel, Lijun Wang**

**9:20 Paper 640e:** Targeting Techniques for Efficient Biomass Gasification — **Saneliswa Magagula, Baraka Celestin Sempuga, Neil Thomas Stacey**

**9:40 Paper 640f:** Study of Effect of Reaction Conditions on the Hydrothermal Liquefaction Reaction Followed By Steam Reforming of the Liquefaction Liquid — **Haider Niaz, Yong Beom Park, J. Jay Liu, Hee-Chul Woo**

#### (641) Adsorbent Materials: MOFs I

**Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 305

T. Grant Glover, Chair  
Bin Mu, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**12:30 Paper 641a:** Enhancement of Adsorbed Natural Gas Storage in Defect-Engineered MOFs during Long-Term Cycling — **Ying Wu, Qibin Xia, Zhong Li, Hongxia Xi, David S. Sholl**

**12:55 Paper 641b:** Investigation of Missing-Cluster Defects in UiO-66 and Ferrocene Deposition on Defective Sites for  $\text{O}_2/\text{N}_2$  Separation — **Bohan Shan, Bin Mu**

**1:20 Paper 641c:** Chemical Potential Difference between the Large and Narrow Pore Forms of MIL-53 (Al) — **Rushik G Bhandokar, Dustin Bowden, Satyanarayana Edubilli, Orhan Talu, Sasiidhar Gumma**

**1:45 Paper 641d:** Unveiling Metal Organic Framework for Handling Indoor and Gas Containing Humidity — **Youssef Belmabkhout**

**2:10 Paper 641e:**  $\text{CO}/\text{N}_2$  Separation Using MOFs: Investigation of the Role of Metal Type and Metal Density — **Arwyn Evans, Abdulmalik Ajenifuja, Matthew Cummings, Salman Shahid, Donato Decarolis, Andi Tao, Megan Jobson, Martin Attfield, David Fairen-Jimenez, Klaus Hellgardt, Camille Petit**

**2:35 Paper 641f:** Towards Systematic Assessment of Porous Adsorbents for Post-Combustion  $\text{CO}_2$  Capture Via Multiscale Simulation Strategies — **Amir H. Farmahini, Shreenath Krishnamurthy, Daniel Friedrich, Stefano Brandani, Lev Sarkisov**

## (642) Advanced Treatment for Water Reuse and Recycling II

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 319

Jeffrey McCutcheon, Chair

Sage R. Hilbel, Co-Chair

**Sponsored by:** Water

**12:30 Paper 642a:** An Innovative Microalgae-Bacteria Symbiotic Process for in-Situ Secondary and Tertiary Treatment of Wastewater — **Sheetal Kishor Parakh**, Prashant Praveen, Yen Wah Tong, Kai Chee Loh

**12:45 Paper 642b:** Synergistic Cr(VI) Treatment with *S. Oneidensis*-reduced Metal-Organic Frameworks — **Sarah K. Springthorpe**, Christopher M. Dundas, Benjamin K. Keitz

**1:00 Paper 642c:** Humidification/Dehumidification for Low Cost, Energy Efficient, Zero Liquid Discharge Desalination Using Solar Thermal Sources — **Ali Hassanzadeh**, Roland Winston, James W. Palko

**1:15 Paper 642d:** Improving Speed and Efficiency of Global Sensitivity Analysis Using Metamodeling-Based Approach: A Case Study on Wastewater Treatment Plant Modeling — **Resul Al, Chitta Ranjan Behera**, Alexandr Zubov, Krist V. Germaey, Gürkan Sin

**1:30 Paper 642e:** Rational Design of Tailor-Made Threshold Scale Inhibitor Dendrimers and Dendrons — **Amir Sheikhi**, Theo G. M. van de Ven, Ashok Kakkar

**1:45 Paper 642f:** Biochar-Alginate Novel Composite Adsorbent: Synthesis Characterisation and Application in Water and Wastewater Treatment — **Subrata Biswas**, Tushar Kanti Sen, Bhim Charan Meikap

## (643) Advances in Metabolic Engineering of Autotrophic Organisms

Thursday, Nov 1, 12:30 PM

Westin Convention Center, Westmoreland East

Nanette R. Boyle, Chair

Robert Jinkerson, Co-Chair

Arul Varman, Co-Chair

Hsien-Chung Tseng, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 643a:** Transcriptional Regulators for Predictable and Precise Gene Expression in the Metabolically Versatile *Rhodospseudomonas Palustris* CGA009 — **Cheryl Immethun**, Dianna Long, Rajib Saha

**12:48 Paper 643b:** Methane-Limited Vs Oxygen-Limited Growth of *Methylobacterium Buryatense* 5GB1: a Systems Approach — **Kyle Stone**, Q. Peter He, Jin Wang

**1:06 Paper 643c:** Model-Guided Engineering of Cyanobacteria for Stable, High-Yield Biofuel Production — **Hugh Purdy**, Jennifer Reed

**1:24 Paper 643d:** Development of Genetic Tools for the Biomining Bacterium, *Acidithiobacillus Ferrooxidans* — **Yuta Inaba**, Timothy Kernan, Indrani Banerjee, Alan C. West, Scott Banta

**1:42 Paper 643e:** Model-Guided Metabolic Engineering of Increased 2-Phenylethanol Production in Plants — **Shaunak Ray**, Joseph Lynch, Clint Chapple, Natalia Dudareva, John A. Morgan

**2:00 Paper 643f:** Developing Genome-Scale Whole-Plant Models for Poplar (*Populus deltoides*) and Switchgrass (*Panicum virgatum*) — **Patrick F. Suthers**, Debolina Sarkar, Costas Maranas

**2:18 Paper 643g:** Enabling More Predictive Modeling of Photoautotrophic Growth Using a Multi-Scale Multi-Paradigm Approach — **Nanette R. Boyle**

## (644) Alternative Fuels and Enabling Technology II

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 323

Seiya Hirohama, Chair

Rajesh Khare, Co-Chair

Nevin Gereke, Co-Chair

**Sponsored by:** Alternate Fuels and New Technology

**12:30 Paper 644a:** Effect of Interfacial Heterogeneity on Heavy Oil Desorption — **Yun Bai**, Lin He, Hong Sui, Xingang Li

**12:55 Paper 644b:** Synthesis and Application of Amino Acid Ionic Liquid-Based Deep Eutectic Solvents for Oil-Carbonate Mineral Separation — **Ning Kang**, Lin He, Hong Sui, Zisheng Zhang

**1:20 Paper 644c:** Geothermal Sludge-Derived Calcined Sodium Silicate As Heterogeneous Catalyst for Biodiesel Production from Waste Cooking Oil — **Ichsan Dwi Nugraha**

**1:45 Paper 644d:** Performance of Microemulsions As an Alternative Fuel in Constant Speed Diesel Engine — **Ilyman Abrar**, Ashok N. Bhaskarwar

**2:10 Paper 644e:** Contribution of Ignition Timing Variation to the Greenhouse Gas Emission and Coolant Performance in Spark Ignition Engine — **Esam I. Jassim**, Bashar I. Jasem

**2:35 Paper 644f:** Experimental Study of a Fluidized Bed Reactor for Obtaining Biodiesel from *Jatropha curcas* Oil By Means of Immobilized Enzymes: Stage 1: Characterization of Lipase — **Boris Guzman Martinez**, Roberto Limas Ballesteros, Jin An Wang, Lifang Chen

## (645) Application of Process Modelling to Pharmaceutical Process Design and Scale-up

Thursday, Nov 1, 12:30 PM

Westin Convention Center, Fayette

Mary T. am Ende, Chair

Michael L. Hoffman, Co-Chair

Mehrdad Kheiripour, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**12:30 Paper 645a:** Importance of the Rheological Characterization on the Spray Performance of Pharmaceutical Formulations — **Tiago Porfirio**, Rui C. Silva, João Vicente, Viriato Semião

**12:51 Paper 645b:** Scaling up and Optimization of Process Parameters for a Spray Drying Plant Using Mechanistic Modelling — **Sridevi Challa**, Yakoob Sardar Mohammed, Veera Pratap Reddy Kasina, RaviChandra Palaparthi, Srividya Ramakrishnan, Ravi Kumar Gorle

**1:12 Paper 645c:** Industrial Application of Mechanistic Model for Fluid-Bed Granulation for Technology Transfer and Design Space Exploration — **David R. Ochsenbein**, Matthew W. Billups, Bingbing Hong, Elisabeth Schäfer, Alexander J. Marchut, Olav Lyngberg

**1:33 Paper 645d:** Practical Application of a Mechanistic Model for Twin Screw Granulation for Pharmaceutical Process Development — **Dana Barrasso**, Leonor Rosa, Sean K. Bermingham, Gavin Reynolds

**1:54 Paper 645e:** Ibrance® Capsule Commercial Process: Designed for Robustness — **Mary T. am Ende**, John Kresevic, Matthew P. Mullarney, Holger Schlack, William R. Ketterhagen

**2:15 Paper 645f:** Application of Integrated Modeling Approach for Quality-By-Design (QbD) Process Development of Lyophilization — **Kushal Sinha**, Tong Zhu, Ehab Moussa, Deliang Zhou, Madeleine Witting, Nandkishor Nere, Sherwin Shang, Mario Hirth, Martin Bultmann, Nupur Dutta, Ted Sharp, Feroz Jameel, Martin Gastens, Alina Alexeenko

**2:36 Paper 645g:** Drug Product Process Modeling — **Mary T. am Ende**, William R. Ketterhagen, Andrew Prpich, Salvador Garcia-Muñoz, Pankaj Doshi, Rahul Bharadwaj

## (646) Application of Solid-Liquid Separation Technologies to Produced Water

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 301

Olayinka I. Ogunsola, Chair

Erica Folio, Co-Chair

**Sponsored by:** Fluid-Particle Separations

**12:30 Paper 646a:** Treatment Approaches for Produced Water Re-Use and Surface Discharge — **Madison Wenzlick**, Alexandra Hakala, Nicholas Siefert

**12:55 Paper 646b:** Advanced Supercritical Water-Based Process Concepts for Treatment and Beneficial Reuse of Brine Generated By Oil/Gas Production — **Jason Trembly**, Chad Able, David Ogden

**1:20 Paper 646c:** Transport of Earth Alkaline Elements in Produced Water through Reactive Porous Media — **Zi Ye**, Valentina Prigiobbe

**1:45 Paper 646d:** Permian & Anadarko Basin Produced Water Recycling: Keys to Success — **J. Daniel Arthur**

## (647) Atomically Dispersed Supported Metal Catalysts I

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 406

Ning Yan, Chair

Nicholas Brunelli, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 647a:** Modeling of Single Atom Catalysis for CO Oxidation — **Konstantinos Alexopoulos**, Dionisios G. Vlachos

**12:50 Paper 647b:** Iridium and Rhodium Pair-Site Catalysts Supported on MgO — **Erjia Guan**, Bruce C. Gates

**1:10 Paper 647c:** Predicting the Single-Site CO Oxidation Reactivity Trends on a Well-Defined Copper Oxide Film — [Kyle Groden](#), [Alex C. Schilling](#), [Alyssa Hensley](#), [Andrew Therrien](#), [E. Charles H. Sykes](#), [Jean-Sabin McEwen](#)

**1:30 Paper 647d:** Correlation between Atom-Support Interaction and Catalyst Stability & Activity: Implications from a Series of Heteropoly Acids Based Pt1 Catalysts — [Ning Yan](#)

**1:50 Paper 647e:** Strong Electrostatic Adsorption and Cryogenic IR Spectroscopy As a General Synthesis and Characterization Approach for Oxide Supported Single Atom Rh Catalysts — [Chithra Asokan](#), [Phillip Christopher](#)

**2:10 Paper 647f:** Theoretical Insights on Boron Nitride-Supported Sub-Nanometer Pd6 Clusters for Formic Acid Decomposition: The Effect of Defects — [Roberto Schimmenti](#), [Manos Mavrikakis](#)

**2:30 Paper 544by:** Atomically Dispersed Pt and Pd in Small-Pore Chabazite: Synthesis, Characterization and Application — [Konstantin Khivantsev](#), [Libor Kovarik](#), [Nicholas Jaegers](#), [Jonathan C. Hanson](#), [Franklin \(Feng\) Tao](#), [Hristiyan A. Aleksandrov](#), [Georgi N. Vayssilov](#), [Yong Wang](#), [Feng Gao](#), [Janos Szanyi](#)

#### (648) Atomistic and Molecular Modeling and Simulation of Polymers

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 330

Li Xi, Chair  
Guozhen Yang, Co-Chair

**Sponsored by:** Polymers

**12:30 Paper 648a:** Deformation and Yield in Semicrystalline Polymers — [Gregory C. Rutledge](#), [Sanghun Lee](#), [Jun Mo Kim](#), [Shuze Zhu](#)

**1:00 Paper 648b:** Computing Mechanical Properties of Elastomers Under Multiaxial Deformation Using Molecular Modeling — [Suvrajyoti Kar](#), [Julie Cuddigan](#), [Michael L. Greenfield](#)

**1:15 Paper 648c:** Molecular Modeling of Mechanical Properties of Semicrystalline Polymer Fibers — [Amulya K. Pervaje](#), [Melissa A. Pasquinelli](#), [Saad A. Khan](#), [Erik E. Santiso](#)

**1:30 Paper 648d:** Predicting Nematic Coupling of Polybutadiene Using Atomistic Molecular Dynamic Simulations — [Shreya Shetty](#), [Enrique D. Gomez](#), [Scott T. Milner](#)

**1:45 Paper 648e:** A Multiscale Modeling Approach to Characterizing Structural and Transport Properties in Diblock Copolymer Polymerized Ionic Liquids — [Jordan R. Keith](#), [Venkat Ganesan](#)

**2:00 Paper 648f:** Applying Protracted Colored Noise Dynamics to Dramatically Increase the Simulation Efficiency of Linear Polymer Systems — [Peter J. Ludovice](#), [Andrew Peters](#), [Benjamin Nation](#), [Clifford L. Henderson](#)

**2:15 Paper 193af:** An Atomistic Evaluation of the Compatibility and Plasticization Efficacy of Phthalates in Poly(vinyl chloride) — [Dongyang Li](#), [Kushal Panchal](#), [Li Xi](#)

**2:30 Paper 648h:** Zwitterionic Contribution to the Hydration Lubrication Dynamics of Poly(2-methacryloyloxyethyl phosphorylcholine) — [Justin Gilmer](#), [Christoph Klein](#), [William L. Rousell](#), [Chris Iacovella](#), [Peter T. Cummings](#), [Clare McCabe](#)

**2:45 Paper 648i:** Protein Stabilization in Non-Native Solvents with Random Copolymers — [Trung Nguyen](#), [Monica Olvera de la Cruz](#)

#### (649) Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries I

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 325

Shijie Liu, Chair  
Xiao Zhang, Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**12:30 Paper 649a:** Novel Dihydrogen-Bonding Deep Eutectic Solvents: Pretreatment of Rice Straw for Butanol Fermentation Featuring Enzyme Recycling and High Solvent Yield — [Guochao Xu](#)

**12:51 Paper 649b:** Effect of Distinctive Detoxification on Inhibitors Removal and Butanol Fermentation of Poplar Prehydrolysates — [Yu Zhang](#), [Maobing Tu](#), [Changlei Xia](#)

**1:12 Paper 649c:** Increased Lactic Acid Production in Fermentation Process from Woody Biomass and Its Kinetic Modelling — [Jiaqi Huang](#), [Shijie Liu](#)

**1:33 Paper 649d:** Carbon-Based Solid Acid Pretreatment in Corn cob Saccharification: Specific Xylose Production and Efficient Enzymatic Hydrolysis — [Wei Qi](#)

**1:54 Paper 649e:** Hydrolysis of Cellulose and Its Adsorption Performance on Heavy Metal Ions — [Yaoyao Wang](#), [Shijie Liu](#)

#### (650) Biomacromolecular Gels

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 326

Jessica Schiffman, Chair  
Erick S. Vasquez, Co-Chair

**Sponsored by:** Polymers

**12:30 Paper 650a:** Humidity Tempering of and Cytokine Release from Polyelectrolyte Complexes — [Xuejian Lyu](#), [Ivan Ding](#), [Amy M. Peterson](#)

**1:00 Paper 650b:** Biopolymer-Derived Tough Homogeneous Polyelectrolyte Complexes Hydrogels As the Potential Electro-Responsive Actuators — [Qingye Liu](#), [Ziye Dong](#), [Zhenya Ding](#), [Wei Li](#)

**1:15 Paper 650c:** Photolithographically Assembled Polyelectrolyte Complexes As Shape-Directing Templates for Thermoreversible Gels — [Kunal Choudhuri](#), [Udaka K. de Silva](#), [Vincent Huynh](#), [Ryan G. Wylie](#), [Yakov Lapitsky](#)

**1:30 Paper 650d:** Elastomeric and Mechanoresponsive Polymer Matrix Composites: Design, Synthesis, and Performance — [Matthew D. Green](#), [Meng Wang](#)

**1:45 Paper 650e:** Engineering Nucleoporin-Inspired Hydrogels to Control Biomolecular Transport — [Danielle J. Mai](#), [Yun Jung Yang](#), [Allison Huske](#), [Thomas J. Dursch](#), [Bradley D. Olsen](#)

**2:00 Paper 650f:** Physically Crosslinked DNA-Based Injectable Hydrogels — [Sayantani Basu](#), [Settimio Pacelli](#), [Arghya Paul](#)

**2:15 Paper 650g:** Characterizing the Physical Properties of Polyampholyte Hydrogels with Different Ethylene Glycol Cross-Linkers — [Emily Mariner](#), [Matthew T Bernards](#)

**2:30 Paper 650h:** Development of Visible-Light Responsive and Mechanically Enhanced "Smart" Ucast Interpenetrating Polymer Network Hydrogels — [Yifei Xu](#), [Onkar Ghag](#), [Philip Sitterle](#), [Hongyu Yu](#), [Hanqing Jiang](#), [Lenore L. Dai](#)

**2:45 Paper 650i:** Main-Chain Liquid Crystalline Networks Synthesized Using Click Chemistry — [Yongjian Wang](#), [Kelly A. Burke](#)

#### (651) Biomass Characterization, Pretreatment, and Fractionation I

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 324

Xuejun Pan, Chair  
Justinus Satrio, Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**12:30 Paper 651a:** Introduction of Self-Steam Explosion Pretreatment Technology for Wet Biomass — [Dedy Eka Priyanto](#)

**12:55 Paper 651b:** Optimization of Sequential Biomass Pretreatment Using Lignin-Modifying Enzymes and Ionic Liquids — [Michael Doane](#), [Blake A. Simmons](#)

**1:20 Paper 651c:** Non-Equilibrium Plasma Pretreatment of Biomass for Enhanced Conversion — [Lusi A. Haiyang Hu](#), [Hui Hu](#), [Xianglan Bai](#)

**1:45 Paper 651d:** Effect of Aromatic Additives on Dilute Acid Pretreatment of Aspen — [Yequan Sheng](#), [Maobing Tu](#), [Changlei Xia](#)

**2:10 Paper 651e:** Fractionation, Conversion, and Valorization of Lignocellulosic Biomass in Inorganic Ionic Liquid (molten salt hydrate) — [Xuejun Pan](#)

**2:35 Paper 651f:** Are Lignocellulosic Feedstocks Commercially Relevant to Make Pure Sugars for Chemical Catalytic Upgrading? — [Sampath Gunukula](#), [Hemant P. Pendse](#), [Thomas J. Schwartz](#), [Adriaan van Heiningen](#), [William J. DeSisto](#), [M. Clayton Wheeler](#)

#### (652) Biomaterials in Industry and the Clinic

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 328

Julianne L. Holloway, Co-Chair  
Sam N. Rothstein, Co-Chair

**Sponsored by:** Biomaterials

**12:30 Paper 652a:** Two Decades of Commercializing Biomaterials: The Good, the Bad, and the Ugly — [Thomas J. Webster](#)

**1:06 Paper 652b:** Cancer Immunotherapy with PLGA Microparticles: Product Development from Benchtop through IND-Enabling Studies — [Sam N. Rothstein](#)



**1:24 Paper 652c:** 3D Printed Absorber for Capturing Chemotherapy Drugs before They Are Released in the Body — **Hee Jeung Oh**, Mariam Aboian, Michael Yi, Jacqueline Maslyn, Whitney Loo, Xi Jiang, Dilworth Parkinson, Mark Wilson, Terilyn Moore, Colin Yee, Gregory Robbins, Florian Barth, Joseph M DeSimone, Steven W. Hettis, Nitash P. Balsara

**1:42 Paper 652d:** Leveraging Surface Science of Biomaterials for Improving Oral Health Outcomes — **Latrish K. Petersen**, Daniel Queiroz, Patricia Golas, Deepak Sharma, Benjamin Serbiak, Tara Furre, Tony McGuire, Carolyn Mordas, Robert J. Gambogi

**2:00 Paper 652e:** Development of a Controlled Release Platform for Topical Ocular Drug Delivery — **Morgan Fedorchak**

**2:18 Paper 652f:** Using Solid-State NMR As a Means to Quantify Protein Integration in Hydrogel Contact Lens Materials — **Noelle I. Rabiah**, Charles W. Scales, Gerald G. Fuller, Lynette S. Cegelski

**2:36 Paper 652g:** Elucidating the Effects of an IL-4 Eluting Coated Polypropylene Mesh in a Novel Rabbit Surgical Model of Pelvic Reconstruction — **Aimon Iftikhar**, Alexis Nolfi, Bryan Brown

### (653) Catalysis with Microporous and Mesoporous Materials IV: Conversion of Renewables, Natural Gas, and Petroleum

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 404

Michele L. Sarazen, Chair  
Sarika Goel, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 653a:** Investigation of the Formaldehyde-Isobutene Prins Condensation over MFI Zeolites — **Efterpi Vasiliadou**, Sha Li, Stavros Caratzoulas, Raul F. Lobo

**12:50 Paper 653b:** 3D-Printed Monoliths of MFI Zeolite with Hierarchical Porosity for Methanol-to-Olefin Reaction — **Xin Li**, Ali Rowanaghi, Fateme Rezaei

**1:10 Paper 653c:** Influence of Confining Environment Polarity and Active Site Structure on Ethanol Dehydration Catalysis By Lewis Acid Zeolites — **Jason S. Bates**, Rajamani Gounder

**1:30 Paper 653d:** Dehydroaromatization of Ethylene over Bifunctional Lewis-Brønsted Acid Pairs in Ag-ZSM-5 — **Hari Thirumalai**, Unmesh Menon, Yunwen Zhou, Jeffrey D. Rimer, Lars C. Grabow

**1:50 Paper 653e:** Ethylene Oligomerization to Select Oligomers on Ni<sup>2+</sup>-Containing ETS-10 — **Jay Thakkar**, Xinyang Yin, Xueyi Zhang

**2:10 Paper 653f:** Hydrodeoxygenation of Biomass Pyrolysis Vapors Using Metal Supported USY Zeolite — **Julia A. Valla**, David P. Gamliel

**2:30 Paper 653g:** Zeolite Bead Heterogeneous Catalysts for Biomass Upgrading in Monophasic and Biphasic GVL Solvent Systems — **Joelle Romo**, Tara Sundsted, Ting Wu, Jolie Lucero, Moises Carreon, Jesse Q. Bond, Stephanie G. Wettstein

### (654) Catalytic Hydrocarbon Processing I: Oxidative Upgrading of Light Hydrocarbons

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 403

William W. Lonergan, Chair  
Nan Yi, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 654a:** Investigating Solid Oxide Membrane Reactors for Direct Methane Conversion to Ethylene and Ethane By Oxidative Coupling — **Valentina Omoze Igenegbai**, Randall J. Meyer, Suljo Linic

**12:50 Paper 654b:** Tandem Reactions of CO<sub>2</sub>-Assisted Light Alkane Dehydrogenation and Aromatization — **Elaine Gomez**, Jingguang G. Chen

**1:10 Paper 654c:** Investigation of the Effect of Pre-Treatment Methods on the Reactivity of Methane, Steam and Oxygen over NiO/CeZr1-XO<sub>2</sub> — **Yimeng Lyu**, Carsten Sievers

**1:30 Paper 654d:** Influence of Confinement in Pores of M1 Phase Mixed Oxides on Selective Oxidative Dehydrogenation of Ethane — **Annamalai Leelavathi**, Yilang Liu, Sopuruchukwu Ezenwa, Yanliu Dang, Steven Suib, Prashant Deshlahra

**1:50 Paper 654e:** Alkali-Promoted Mixed Oxide Redox Catalysts for Oxidative Dehydrogenation of Ethane in a Cyclic Redox Scheme — **Fanxing Li**, Yunfei Gao

**2:10 Paper 654f:** Propane Oxidative Dehydrogenation Catalyzed By Iodine, Bromine, and Halide Salts — **David Chester Upham**, Henrik Kristoffersen, Zachary Snodgrass, Michael Gordon, Eric W. McFarland, Horia Metiu

**2:30 Paper 654g:** Atomistic Design of Propylene Epoxidation Catalysts — **Zheng Lu**, Yong Qin, C. Heath Turner, Yu Lei

### (655) Catalytic Processing of Fossil and Biorenewable Feedstocks I: Acids, Alcohols, and Polyols

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 405

Julia A. Valla, Chair  
Steven Crossley, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 655a:** Catalytic Etherification of Glycerol to Glycerol Oligomers in the Presence of Alumina Supported Ca/Sr Mixed Oxides — **Yi-Chen Shih**, Bing-Hung Chen

**12:48 Paper 655b:** The Role of Copper Stability in Selectively Condensation of Ethanol to Higher Alcohols — **Mond Guo**, Karthikeyan K. Ramasamy

**1:06 Paper 655c:** Effects of Alloying Pd and Cu on Tandem Dehydrogenation-Aldol Condensation Reactions — **Konstantinos A. Goulas**, Yuying Song, Lars C. Grabow, Dean Toste

**1:24 Paper 655d:** Lubricant Base Oils Production from Biomass — **Sibao Liu**, Basudeb Saha, Dionisios G. Vlachos

**1:42 Paper 655e:** Selectivity Control during the One-Pot Conversion of Aliphatic Carboxylic Acids to Linear Olefins through Tandem Hydrogenation/Dehydration — **Jher Hau Yeap**, Bartosz Rozmyslowicz, Jeremy S. Luterbacher

**2:00 Paper 655f:** Mechanism and Kinetics of Isobutene Production over Zirconia-Supported Zinc Oxides — **Julie Rorrer**, Alexis T. Bell, Dean Toste

**2:18 Paper 655g:** Catalytic Upgrading of Sugar-Derived Polyols to Glycols in Absence of Externally Added Hydrogen — **Bin Yin**, Xin Jin, Guangyu Zhang, Hao Yan, Chaohe Yang

**2:36 Paper 655h:** Selective C-C Bond Scission of Primary Alcohols Using Cerium Oxide-Supported Palladium Catalyst — **Tomoo Mizugaki**, Kodai Nitta, Takato Mitsudome, Koichiro Jitsukawa

**(656) Characterization and Measurement in Powder Processing**  
**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 414

Michael Winn, Chair  
Madhusudhan Kodam, Co-Chair

**Sponsored by:** Solids Flow, Handling and Processing

**12:30 Paper 656a:** In-Line Evaluation of Powder Properties during Mixing Processes Using a Drag Force Flow Sensor — **Tim Freeman**, Jamie Clayton, John Yin, Laura Monington, Markus Klink, Bernd Buecker

**12:48 Paper 656b:** Revisiting the Measurement of Powder Permeability Under Applied Load — **Michael Winn**, Benjamin Ennis, Bryan J. Ennis

**1:06 Paper 656c:** Triboelectrification of Insulator Materials in a Humidified Environment — **Erik M. Jensen**, Maria Kezhia D. Rullan, Keith M. Forward

**1:24 Paper 656d:** Bipolar Charging of Polyethylene Powders: Experimental and Modelling Study — **Simon Jantac**, Ladislav Konopka, Matej Vrzáček, Jaromir Podedic, Juraj Kosek

**1:42 Paper 656e:** Evaluating Electrostatic Charging of Powders - the Challenges — **Tim Freeman**, Jamie Clayton, John Yin, Rajeev Dattani

**2:00 Paper 656f:** Powder Permeability As a Measurement Surrogate for Triboelectric Charging — **Benjamin Ennis**, Michael Winn, Naseem Jibrin, Bryan J. Ennis

**2:18 Paper 656g:** Influence of Powder Mixture Composition on Macroscopic Powder Properties — **Eva Faulhammer**, Johannes G. Kheinast, Sara Fathollahi

**2:36 Paper 656h:** Effect of Intrinsic Materials Properties on the Mechanical and Rheological Behavior of API Agglomeration in Agitated Filter Dryers — **Yu Jin Shin**, Raimundo Ho, Nandkishor K. Nere, Kushal Sinha, Prashant Kumar, Laurie Minar, John G. Gaertner, Shailendra Bordawekar, Ahmad Sheikh



Information as of September 25, 2018. An up-to-date program is available at [aiche.org/annual](http://aiche.org/annual) or on the AICHEvents app.

## (657) Chromatographic Separations and SMB

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 309

Yoshiaki Kawajiri, Chair  
Reza Haghpahan, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**12:30 Paper 657a:** Model Predictive Control of 4-Zone Simulated Moving Bed Chromatography for the Separation of Bicalutamide Enantiomers: Experimental Validation — **Ju Weon Lee, Andreas Seidel-Morgenstern**

**12:55 Paper 657b:** Separation of Anhydrosugars and Phenolic Species in a Fast Pyrolysis Aqueous Product Stream Using Resin Adsorbents and Simulated Moving Bed Technology — **John P. Stanford, Andrew Friend, Haoqin Zhou, Marjorie R. Rover, Ryan G. Smith, Robert C. Brown**

**1:20 Paper 657c:** Constant-Pattern Design of Displacement Chromatography — **David M. Harvey, Hoon Choi, Nien-Hwa Linda Wang**

**1:45 Paper 657d:** ZIF-8 As an Efficient Adsorbent for Ethane/Ethylene Separation By Gas Phase Simulated Moving Bed — **Vanessa F. D. Martins, Ana M. Ribeiro, Pavel Kortunov, Alexandre Ferreira, Alirio E. Rodrigues**

**2:10 Paper 657e:** Aromatics/Alkanes Separation: Simulated Moving Bed Process Model Development By a Concurrent Approach and Its Validation in a Mini-Plant — **Siwei Guo, Shaowei Yang, Krishna Chandran Jayachandrababu, Pranav S. Vengsarkar, Yoshiaki Kawajiri, Sankar Nair**

## (658) Complex and Networked Chemical and Biochemical Systems

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 409

Steven M. Abel, Chair  
Mark P. Styczynski, Co-Chair  
Elizabeth Read, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

**12:30 Paper 658a:** On Integration of Feedback Control and Safety Systems for Networked Chemical Processes — **Zhihao Zhang, Zhe Wu, Carlos Garcia, Helen Durand, Panagiotis D. Christofides**

**12:49 Paper 658b:** Manifold Learning for Measurements across Several Sensors: Alternating Diffusion, Data Fusion and Constructing Nonlinear Observers for Complex Chemical Reaction Networks — **David Sroczynski, Felix Dietrich, Mahdi Kooshkbaghi, Seungjoon Lee, Ioannis G. Kevrekidis**

**1:08 Paper 658c:** Emergence of Structural Features in Complex Networks Via Adaptation — **Abhishek Sivaram, Sihyun Lee, Jackson Chen, Meir Retter, Resmi Suresh, Yu Luo, Venkat Venkatasubramanian**

**1:27 Paper 658d:** Modeling the Stochastic Dynamics of Gene Regulatory Networks Using Probabilistic Boolean Networks — **Cameron Gallivan, Elizabeth Read**

**1:46 Paper 658e:** Koptic: A Novel Approach for *in silico* Prediction of Enzyme Kinetics and Regulation — **Wheaton Schroeder, Rajib Saha**

**2:05 Paper 658f:** Lung Immunodynamics during pH1N1 Influenza Virus Infection — **Emily E. Ackerman, Ericka Mochan, Jason E. Shoemaker**

**2:24 Paper 658g:** Understanding the Basal Ganglia Dynamic Transition from the Healthy to the Parkinsonian State — **Joseph Schmalz, Gautam Kumar**

**2:43 Paper 658h:** Dynamic Transcriptomic Profiling of *Scheffersomyces stipitis* Reveals Key Information of Its Gene Regulatory Network at Genome-Scale — **Matthew Hilliard, Thomas Jeffries, Q. Peter He, Jin Wang**

## (659) Data Science in Catalysis I

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 402

Andrew Medford, Chair  
Zachary Ulissi, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 659a:** Knowledge Extraction Via Machine Learning from High-Throughput Catalytic Experiments — **Travis Williams, Katherine McCullough, Jochen Lauterbach**

**12:48 Paper 659b:** Catalyst Characterization from Complex Infrared Spectroscopy: A Machine Learning Approach — **Joshua Lansford, Dionisios G. Vlachos**

**1:06 Paper 659c:** Heterogeneous Catalysis Kinetic Characterization Via Sparse Graphs — **M. Ross Kunz, Yixiao Wang, Zongtang Fang, Andrew Medford, Gregory S. Yablonsky, Rebecca Fushimi**

**1:24 Paper 659d:** Bayesian Experimental Design and Mean Field Microkinetic Modeling of Heterogeneous Catalytic Systems — **Huijie Tian, Srinivas Rangarajan**

**1:42 Paper 659e:** Thermochemistry of Gas-Phase and Surface Species Via Lasso-Assisted Subgraph Selection — **Geun Ho Gu, Petr Plechac, Jonathan Lym, Dionisios G. Vlachos**

**2:00 Paper 659f:** Theoretical Investigation of the Pt Catalyzed Hydrodeoxygenation of Succinic Acid to 1,4-Butanediol — **Wenqiang Yang, Osman Mamun, Andreas Heyden**

**2:18 Paper 659g:** Large-Scale Exploration of Perovskites for Oxygen Evolution Via Adaptive Machine Learning — **Zheng Li, Qinghe Zheng, Noushin Omidvar, Hongliang Xin**

**2:36 Paper 659h:** Prospects for Solving Micro-Kinetic Models with Automatic Differentiation and Regression — **Andrew Medford**

## (660) Emulsions and Foams II

Thursday, Nov 1, 12:30 PM

Omni William Penn Hotel, Conference Center A

Xue Chen, Chair  
Peter J. Beltramo, Co-Chair

**Sponsored by:** Interfacial Phenomena

**12:30 Paper 660a:** Influence of Interfacial Shear Elasticity on Liquid Entrainment in Foam Films — **John M. Frostad, Gigi Lin, Gerald G. Fuller**

**12:45 Paper 660b:** A New Coaxial Capillary Pendant Drop Method to Study the Interfacial Tension and Interfacial Rheology of Double Emulsion Formulations — **Abu Zayed Md Badruddoza, Stephanie V. MacWilliams, Abigail Garver, Damien A. Sebben, Mariam Ibrahim, Sarah Aboelela, Marta Krasowska, Thomas D. Roper, David Beattie, James K. Ferri**

**1:00 Paper 660c:** Investigation of the Spontaneous Emulsification Phenomenon in the Presence of Asphaltenes Using Microfluidics — **Simone Bochner de Araujo, Mathilde Reyssat, Cecile Monteux, Gerald Fuller**

**1:15 Paper 660d:** Microrheology and Structure Evolution of Monodisperse Double Emulsions By Diffusive Wave Spectroscopy (DWS) — **Abu Zayed Md Badruddoza, Stephanie V. MacWilliams, Abigail Garver, Damien A. Sebben, Mariam Ibrahim, Sarah Aboelela, Marta Krasowska, Thomas D. Roper, David Beattie, James K. Ferri**

**1:30 Paper 660e:** Towards Continuously Operated Chemical Reactions in Bicontinuous Systems: Making Robust Strips-Bijels for Microfluidic Applications — **Stephen Boakye-Ansah, Martin F. Haase**

**1:45 Paper 660f:** Viscoelastic Characterisation of an Emulsion Drops Coating Via Capsule Compression — **Matthew Biviano, Joe Berry, Lukas Böni, Peter Fischer, Raymond R. Dagastine**

**2:00 Paper 660g:** Formation and Stability of Foams in Pluronic Solutions for Biomedical Applications — **Joy Baxter, Glenn W. Laub, Nicolas J. Alvarez**

**2:15 Paper 660h:** Supramolecular Oscillatory Structural Forces and Stratification in Micellar Freestanding Films — **Subinuer Yilixiati, Yiran Zhang, Chrystian Ochoa, Vivek Sharma**

**2:30 Paper 660i:** Lattice Boltzmann Simulations of Foam Drainage and Oscillation and Comparison with Experiments on Microfluidically Generated Foams — **Subhabrata Das, Zi-Xiang Tong, Lauren Eberly, Xi Chen, Charles Maldarelli, Ponisseril Somasundaran**

## (661) Energy Sustainability: Challenges and Solutions

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 317

William M. Barrett, Chair  
Vikas Khanna, Co-Chair  
Emre Gençer, Co-Chair

**Sponsored by:** Sustainable Energy

**12:30 Paper 661a:** Renewable Energy Assessment and Its Integration in Angola — **Horcel Menga, Cornelius Mduduzi Masuku**

**12:55 Paper 661b:** Thermo-Economic Optimization of Mechanical Vapor Recompression System for Shale Gas Produced Water Treatment — **Elmira Mohammadi Shamlou, Radisav Vodic, Vikas Khanna**

**1:20 Paper 661c:** Low Temperature Pyrolysis of Discarded Plastics — **Stefaan J. R. Simons, Darem Ahmad, Hussam Jouhara**

**1:45 Paper 661d:** Pelletization of Spent Coffee Grounds — **Angélica Vargas, Juan Carlos Serrato**

**2:10 Paper 661e:** Air Pollution Control: Pyrolysis Based on Waste to Energy Plant — **Nour Khawatmi**

**2:35 Paper 661g:** Measuring Energy Security from a Comprehensive Assessment of Risk in Fuel Supply Chains — **Richard C. Darton, Colin J. Axon**

**(662) Engineering in Cancer Biology and Therapy I: Signaling**  
**Thursday, Nov 1, 12:30 PM**  
Westin Convention Center, Cambria

Samira M. Azarin, Chair  
Roger Harrison, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**12:30 Paper 662a:** Activation of IRE1 $\alpha$  Protein By Palmitate through the Transmembrane Domain and Its Implications in Progression of Cancer — **Amrita Oak, Christina Chan**

**12:48 Paper 662b:** Probing the Role of Cancer Lipid Microenvironment in the Regulation of Notch Cleavage By Gamma-Secretase — **Lane Gilchrist, William Houlihan, Marilia Barros, Yueming Li**

**1:06 Paper 662c:** A Simulation-Based Optimization Approach to Develop Personalized Colorectal Cancer Screening Strategies — **David Young, Selen Cremaschi**

**1:24 Paper 662d:** The Quaternary State of Polymerized Human Hemoglobin Regulates Oxygenation of Breast Cancer Solid Tumors: A Theoretical and Experimental Study — **Donald Belcher, Julia Ju, Jin Hyen Baek, Ayla Yalamanoglu, Paul Buehler, Daniele Gilkes, Andre Palmer**

**1:42 Paper 662e:** Pharmacometabonomics Approach for Early Prediction of Chemotherapy Induced Peripheral Neuropathy — **Parul Verma, Jamie Renbarger, Jodi Skiles, Bruce Cooper, Doraiswami Ramkrishna**

**2:00 Paper 662f:** Single-Cell Tumor Metabolism of Immune Checkpoint Inhibitors Determines Optimal Dosing for This Class of Antibody Therapeutics — **Ian Nessler, Cornelius Cilliers, Greg Thurber**

**2:18 Paper 662g:** Invited Speaker: Systems Biology Approaches for Designing Combination Therapy for Cancer — **Matthew J. Lazzara**

**(663) Fluidization and Fluid-Particle Systems for Energy and Environmental Applications**  
**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 415

Sarah E. Mena, Chair  
Luke Neal, Co-Chair

**Sponsored by:** Fluidization and Fluid-Particle Systems

**12:30 Paper 663a:** CO<sub>2</sub> Capture and Transport Behaviors of Porous Polymer Beads Containing Metal-Organic Frameworks (MOFs) — **Guanhe Rim, Valizadeh Bardiya, Kyriakos Stylianou, Berend Smit, Ah-Hyung Alissa Park**

**12:49 Paper 663b:** Carbon Mineral Sequestration Integrated with the Recovery of Rare Earth Elements from Alkaline Industrial Wastes and Silicate Minerals — **Chengchuan Zhou, Xiaozhou Zhou, Ah-Hyung Alissa Park**

**1:07 Paper 663c:** Two Dimensional Simulation of Carbon Capture Using Amine-Based Solid Sorbents — **Farnaz Esmaeili Rad, Hamid Arastoopour, Javad Abbasian**

**1:25 Paper 663d:** Tribocharging of Bidisperse Particles in Fluidized Beds — **Xiaoyu Liu, Jari Kolehmainen, Ali Ozel, Sankaran Sundaresan**

**1:43 Paper 663e:** Bubble Hydrodynamic Comparison for Geldart Group a and B Materials at Different Fluidization Regimes — **Shyam Sundaram, Ben Freireich, Reddy Karri**

**2:01 Paper 663f:** Coupled CFD-DEM Simulations for Heat-Exchanger Cleaning — **Albert Kim, Jung-Hyun Moon, Joshua Lelemlia Irvine, Hyeon-Ju Kim, Ho-Saeng Lee**

**2:19 Break**

**2:37 Paper 663h:** Cloudy-Zone Modeling of a Gas-Solid Bubbling Fluidized Bed with Liquid Spray — **Sihang Tian, Jingyuan Sun, Xiaoqiang Fan, Yao Yang, Zhengliang Huang, Jingdai Wang, Yongrong Yang**

**(664) Fundamentals of Catalysis II: Hydrogenation in Supported Catalysis**  
**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 401

Taejin Kim, Chair  
Omar A. Abdelrahman, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 664a:** Enhancing the Specific Activity of Metal Oxides Using Transition-Metal Dopants — **Jonathan Lym, Konstantinos Alexopoulos, Jiayi Fu, Weiqing Zheng, Alexander V. Mironenko, Dionisios G. Vlachos**

**12:48 Paper 664b:** First-Principles Kinetic Monte Carlo Simulations of Hydrogen Spillover across the Ru/TiO<sub>2</sub> Interface — **Xiao Li, Lars C. Grabow**

**1:06 Paper 664c:** Design of Multi-Functional Catalytic Interfaces from First Principles: Modelling Water Gas Shift on Pt/MgO — **Pushkar Ghanekar, Jeffrey Greeley**

**1:24 Paper 664d:** Interaction of Furan and Benzene Derivatives with Palladium Nanoparticle Catalysts and the Mechanism of Conversion into Biofuels — **Lesli Mark, J. Will Medlin, Hendrik Heinz**

**1:42 Paper 664e:** Mechanistic Interpretations and Consequences of Hydrogen Spillover in Toluene Hydrogenation Catalysis — **Ari Fischer, Enrique Iglesias**

**2:00 Paper 664f:** Kinetics and Mechanism of Selective C-Cl Hydrogenolysis By Pd/C Catalysts — **Jalal Tavara, Mohammed Al-Gharawi, M. Clayton Wheeler, Thomas J. Schwartz**

**2:18 Paper 664g:** The Influence of Support Acid Sites on Non-Oxidative Dehydrogenation of Ethanol to Acetaldehyde over Supported Cu Catalysts — **Sergei Hanukovich, Phillip Christopher**

**2:36 Paper 664h:** Tuning Catalyst Activity Using Self-Assembled Monolayers — **Lucas Ellis, Jordi Ballesteros Soberanas, Daniel K. Schwartz, J. Will Medlin**

**(665) Gene Regulation Engineering: Medical and Biotechnological Tools and Applications**  
**Thursday, Nov 1, 12:30 PM**  
Westin Convention Center, Westmoreland West-Central

Anushree Chatterjee, Chair  
Lauren Woodruff, Co-Chair  
Albert Keung, Co-Chair

**Sponsored by:** Bioengineering

**12:30 Paper 665a:** Development of a Genetic Toolkit in *Rhodococcus Opacus* PD630 for Reliable and Predictable Gene Expression — **Drew DeLorenzo, William R. Henson, Austin Rottinghaus, Tae Seok Moon**

**12:48 Paper 665b:** Transcriptional Control through Synthetic Genetic Regulation Devices in *Clostridium sensu Stricto* — **Nicholas R. Sandoval, Rochelle Joseph, Nancy Kim**

**1:06 Paper 665c:** Reprogramming of Liver Cell Lines to Definitive Endoderm By Understanding and Re-Engineering Developmental Master Regulatory Gene Circuits (DRGC) — **Saber Meamardoost, Natesh Parashurama**

**1:24 Paper 665d:** mRNA Half-life Predictor: An *in silico* tool for Metabolic Engineers — **Sanjan T.P. Gupta, Gina C. Gordon, Parmeswaran Ramanathan, Brian F. Pfeiffer, Jennifer L. Reed**

**1:42 Paper 665e:** Decoding the Complexity of Metabolite-Responsive Transcriptional Factors: Cross-Talk, Auto-Regulation and Feedback Control — **Peng Xu**

**2:00 Paper 665f:** Engineered Synbiotic Production and Sensing of Butyrate — **Yanfen Bai, Jennifer Saldanha, Fatima Enam, Jo Anne Powell-Coffman, Thomas J. Mansell**

**2:18 Paper 665g:** Rational Antimicrobial Engineering for Combating Multidrug-Resistant Pathogens — **Anushree Chatterjee**

**(666) Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion I**  
**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 310

Megan A. Creighton, Chair  
Carlos Silvera Batista, Co-Chair  
Evan K. Wujcik, Co-Chair

**Sponsored by:** Carbon Nanomaterials

**12:30 Paper 666a:** Electronic Structure of Electron-Irradiated Graphene and Effects of Hydrogen Passivation — **Asanka Weerasinghe, Ashwin Ramasubramaniam, Dimitrios Maroudas**



**12:55 Paper 666b:** Development of a Novel Nanosensor Platform By Noncovalent Surface Engineering of Two-Dimensional Graphene Quantum Dots — **Rebecca Pinals, Sanghwa Jeong, Markita Landry**

**1:20 Paper 666c:** Interpretation of the Far-Infrared Optical Spectrum of SWCNTs and Graphene — **Christiaan Richter, Anthony Dichiara, Karim Rezouali**

**1:45 Paper 666d:** Formation and Thermomechanical Behavior of Nanocomposite Superstructures from Interlayer Bonding in Twisted Bilayer Graphene — **Mengxi Chen, Andre R. Muniz, Dimitrios Maroudas**

**2:10 Paper 666e:** Electrochemically Triggered Nucleation and Growth of Zinc Phosphate Co-Deposited with Amino-Modified Graphene Oxide — **Yuhui Xie Sr., Xinya Zhang Sr.**

**2:35 Paper 666f:** Dispersion Microstructure and Aerogel Properties of Graphene/Manganese Oxide Mixtures and Hybrids — **Fatima Hamade, James G. Radich, Virginia Davis**

**(667) Innovative Technologies to Accelerate and Enhance Drug Discovery, Development, and Manufacturing**

**Thursday, Nov 1, 12:30 PM**  
Westin Convention Center, Somerset

Shane T. Grosser, Chair  
Andreas S. Bommarius, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**12:30 Paper 667a:** Greenness By Design for Pharmaceutical Synthetic Processes — **Jacob Albrecht, Jun Li, Alina Borovika, Martin Eastgate**

**12:51 Paper 667b:** Data Rich Experimentation Methods Towards Immobilized Biocatalysis for Drug Substance Manufacture — **Shane T. Grosser, Jacob H. Forstater**

**1:12 Paper 667c:** Enzyme Deactivation Probed By Non-Isothermal Continuous Activity Assay — **Matthew A. McDonald, Ronald W. Rousseau, Martha A. Grover, Andreas S. Bommarius**

**1:33 Paper 667d:** Removing Endotoxins from *E. coli*-Based Cell-Free Systems: Towards Enabling on-Demand Distributed Production of Therapeutics — **Bradley C. Bundy, Kristen M. Wilding**

**1:54 Paper 667e:** Mechanistic Modeling and Parameter-Adaptive Nonlinear Model Predictive Control of a Microbioreactor — **Moo Sun Hong, Richard D. Braatz**

**2:15 Paper 667f:** Automated *in silico* Crystallization Process Design Using Solubility Models; Web Applications for Visualization and an Overview of a Solvent Selection Workflow — **Jeremy Merritt, Jeffrey Tan, Ravi Ananthula, Roger Rothhaar**

**2:36 Paper 667g:** Computational Fluid Dynamics Boosted Stochastic Modelling for Integrated Quantitative Understanding of API Crystalline Product Manufacturing Process — **Deepak Jain, Joydeep Kant, Vishwanath Dalvi, Channamallikarjun Mathpati**

**(668) Interfacial Phenomena in Electrochemical Systems**

**Thursday, Nov 1, 12:30 PM**  
Omni William Penn Hotel, Conference Center B

Patricia Taboada-Serrano, Chair  
Andrew C. Hillier, Co-Chair

**Sponsored by:** Interfacial Phenomena

**12:30 Paper 668a:** Understanding the Mechanism of Aqueous Metal Oxidation on the Nanoscale: Vacancy Transport, Energy Barriers, and Rate Predictions — **Michael Nathanson, Krishan Kanhaiya, Hendrik Heinz**

**12:48 Paper 668b:** Role of Stefan-Maxwell Fluxes in the Dynamics of Concentrated Electrolytes — **Bhavya Balu, Aditya S. Khair**

**1:06 Paper 668c:** Computational Analysis and Prediction of the Interfacial Structure and Na Storage Mechanism of Carbon Electrodes in an NaClO<sub>4</sub>/Carbonate Electrolyte — **Sungwon Park, Eunsu Paek**

**1:24 Paper 668d:** Stabilizing Electroconvection in Viscoelastic Media — **Alexander Warren, Lynden A. Archer**

**1:42 Paper 668e:** Study of Surface Interactions in Sodium-Ion Batteries Using Modified Carbon Films — **Sophia E. Lee, Maureen H. Tang**

**2:00 Paper 668f:** Continuous, Efficient Control of Electrochemical Phenomena on Back-Gated 2D Electrodes — **Yan Wang, C. Daniel Frisbie**

**2:18 Paper 668g:** Progress Toward a Standardized Electrode/Electrolyte Benchmarking Approach for Redox Flow Batteries — **Tejal Sawant, James R. McKone**

**2:36 Paper 668h:** Electrochemical Synthesis of Organic Nanorods on Gold Nanoparticles Seeds — **Xuecheng Yu, Mohamed Kilani, Guangzhao Mao**

**(669) Lithium and Beyond: Fundamental Advances in High Performance Batteries II**

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 306

Nian Liu, Chair  
Robert J. Messinger, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

**12:30 Paper 669a:** Crystalline Molybdenum & Manganese Compounds As Cathode Materials for Rechargeable Aluminum Batteries — **Robert J. Messinger, Ankur Jadhav**

**12:50 Paper 669b:** Electrodeposition from Electrolytes with Increased Thermal Stability for Magnesium Batteries — **Laura Merrill, Hunter Ford, Colin Brankin, Jennifer Schaefer**

**1:10 Paper 669c:** Understanding the Electrode/Electrolyte Interphase in Magnesium-Ion Electrolytes with Simple Mg Salts — **Rahul Jay, Jian Zhang, Anton Tomich, Audrey Gorostiza, Vincent Lavallo, Juchen Guo**

**1:30 Paper 669d:** Real-Time Insight into the Doping Mechanism of Redox-Active Organic Radical Polymers — **Shaoyang Wang, Fei Li, Alexandra Easley, Jodie L. Lutkenhaus**

**1:50 Paper 669e:** Long-Life Rechargeable Zinc-Air Battery in Lean-Electrolyte Cell Configuration — **Nian Liu, Yutong Wu, Yamin Zhang**

**2:10 Paper 669f:** Understanding the Atomic Interaction between Electrode and Electrolyte for Aqueous Electrochemical Energy Storage — **Xiaowei Teng**

**2:30 Paper 669g:** High Energy Density Solid State Li Batteries Using a Trilayer Oxide Architecture — **Dennis McOwen, Eric D. Wachsmann, Liangbing Hu, Shaomao Xu, Lei Zhang**

**2:50 Paper 669h:** Computational Study of Lithium Nucleation Tendency in Solid Electrolytes — **Hong-Kang Tian, Yue Qi**

**(670) Mechanics, Structure, and Properties in Polymers**

**Thursday, Nov 1, 12:30 PM**  
David L. Lawrence Convention Center, 331

Santanu Kundu, Chair  
Gregory B. McKenna, Co-Chair

**Sponsored by:** Polymers

**12:30 Paper 670a:** Chemical Heterogeneity in Interfacial Layers of Polymer Nanocomposites — **Pinar Akcora**

**1:00 Paper 670b:** Nonlinear Mechanics of Polymer Glasses: Mechanical Hole-Burning Spectroscopy — **Satish Mangalana, Gregory B. McKenna**

**1:15 Paper 670c:** Study on Linear Viscoelastic Relaxation of Polymers Near and Above Glass Transition — **Yelin Ni, Grigori A. Medvedev, James M. Caruthers**

**1:30 Paper 670d:** Tuning the "Drawability" of Ultra-High Molecular Weight Polyethylene Fibers — **Christopher Henry, Nicolas J. Alvarez, Giuseppe Palmese**

**1:45 Paper 670e:** Composites Comprising Shear-Thickening Fluids and Polymeric Nanofibers — **Behzad Nazari, Jianyi Du, G. C. Rutledge**

**2:00 Paper 670f:** Comparison of Hypervelocity Impact (HVI) Effects in Ultra-High Molecular Weight Polyethylene (UHMWPE) and Poly(methyl methacrylate) (PMMA) — **M. Hunter Bowering, Charles U. Pittman Jr., Thomas E. Lacy Jr., Santanu Kundu**

**2:15 Paper 670g:** Interrelations between Segmental and Chain Dynamics in the Glass Formation Range of Bulk and Nanoconfined Polymers — **Jui-Hsiang Hung, Jayachandra Hari Mangalana, David S. Simmons**

**2:30 Paper 670h:** Necking and Drawing of LLDPE/Seps Rubber Bilayer Laminates — **Rahul Ramachandran, Sankaran Hariharakrishnan, Ronald Fortunato, Steven Abramowitch, Spandan Maiti, Sachin Velankar**

**2:45 Paper 670i:** Relating Mechanics to Chain-Level Architecture in Glassy Crosslinked Polymers — **Robert M. Elder, Timothy W. Silk**

## (671) Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 307

Liangliang Huang, Chair  
Shuangliang Zhao, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**12:30 Paper 671a:** Thermodynamics of Two-Dimensional Systems — **Keith E Gubbins**

**12:45 Paper 671b:** Trade-Off between  $\text{CO}_2/\text{CH}_4$  Membrane Permeability and Selectivity: Mesoscale Insights from Molecular Simulation — **Xiaohua Lu**

**1:00 Paper 671c:** Isobaric Vapor-Liquid Equilibrium of Monoterpene + Sesquiterpene System at Normal Pressure — **Guangyan Yao, Linlin Wang, Xiaopeng Chen, Dankui Liao, Xiaojie Wei, Jiezhen Liang, Zhangfa Tong**

**1:15 Paper 671d:** Reaction Density Functional Theory and Its Application to Reactions in Aqueous Solution — **Shuangliang Zhao, Weiqiang Tang, Cheng Cai, Honglai Liu**

**1:30 Paper 671e:** Curvature Dependence of Henry's Law Constant and Non-Ideality of Gas Equilibrium for Highly Curved Vapor-Liquid Interfaces — **Xian Wang, Zhenjiang Guo, Xianren Zhang**

**1:45 Paper 671f:** Nanostructured Photoelectrodes for Enhanced Charge Carrier and Mass Transfer in Solar Water Splitting — **Zhibin Luo, Chengcheng Li, He Li, Tuo Wang, Jinlong Gong**

**2:00 Paper 671g:** Dynamic Interfacial Tension during Droplet/Bubble Generation at Microchannel Junctions - an Important Mesoscale Scientific Issue in Multiphase Microflow Study — **Kai Wang, Antoine Riaud, Hao Zhang, Guangsheng Luo**

**2:15 Paper 671h:** Modeling of Interfacial Behaviors of Isobutane Alkylation with 2-Butene Catalyzed By Sulfuric Acid/Brønsted Acidic Ionic Liquid — **Weizhong Zheng, Piao Cao, Weizhen Sun, Ling Zhao**

**2:30 Paper 671i:** Computational Modeling of Thermal Diffusion at the Mesoscale — **Joel G. Christenson, Matthew P. Kroonblawd, Ronald J. Phillips**

**2:45 Paper 671j:** Translocation Energy Calculation on Human  $\beta$  Defensin Type 3 through Bacterial Lipid Membranes — **Rabeta Yeasmin, Liquan Zhang**

## (672) Micro- and Nano-Scale Technologies in Life Sciences

Thursday, Nov 1, 12:30 PM

Westin Convention Center, Washington

Vamsi K. Yadavalli, Chair  
Mario Moisés Alvarez, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**12:30 Paper 672a:** Injectable, Brain-Interfaced Optofluidic Device for Programmable Fluid Delivery and Optogenetics — **Yi Zhang, Philipp Gutruf, Daniel Castro, Michael R. Bruchas, John A. Rogers**

**12:48 Paper 672b:** Engineering DNA Gates for Extensible, Multiplexed Cell Sorting — **Shreyas Dahotre, Yun Min Chang, Andreas Wieland, Samantha Stammen, Gabriel Kwong**

**1:06 Paper 672c:** Nanoscale Surface Patterning of Multiple Proteins Using Photoactivation — **Kevin Metcalf, Shengwang Zhou, Milan Mrksich**

**1:24 Paper 672d:** Dual Near Infrared Two Photon Microscopy for 3D Imaging of Biological Systems — **Ian McFarlane, Jackson Travis Del Bonis-O'Donnell, Ralph Page, Abraham Beyene, Eric Tindall, Markita Landry**

**1:42 Paper 672e:** Single Particle Virus Isoelectric Point Determination with Chemical Force Microscopy — **Xue Mi, Pratik Joshi, Emily Bromley, Fei Long, Caryn L. Heldt**

**2:00 Paper 672f:** Continuous 3D Chaotic Printing: Using the Chaotic Flow Induced By a Kenics Mixer to Continuously Fabricate Complex Micro- and/or Nanostructure at High Resolution — **Maria Diaz de Leon-Derby, Carolina Chavez-Madero, Mohamadmahdi Samandari, Christian Carlos Mendoza-Buenrostro, Rute Fabiana Martins-Fernandes, Everardo González-González, Mario Moisés Alvarez, Grissel Trujillo-de Santiago**

**2:18 Paper 672g:** Invited Speaker: Electrolyte Gated Transistors with Floating Gates As Biosensors — **C. Daniel Frisbie**

## (673) Mixed-Matrix Materials for Gas Separation

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 303

Zachary Smith, Co-Chair  
Bin Mu, Co-Chair  
Michele Galizia, Co-Chair

**Sponsored by:** Membrane-Based Separations

**12:30 Paper 673a:** Atomistic Investigation of Polymer-MOF Interfaces in Mixed Matrix Membranes — **Marcel Balcik, S. Birgül Tanteekin-Ersolmaz, M. Gökçug Ahunbay**

**12:51 Paper 673b:** Microscopic Gas Diffusion inside ZIF-11 Crystals Dispersed in Different Polymers to Form Mixed Matrix Membranes — **Evan M. Forman, Amineh Baniani, Lei Fan, Kirk J. Ziegler, Erkang Zhou, Fengyi Zhang, Ryan Lively, Sergey Vasenkov**

**1:12 Paper 673c:** Tailoring Separation Properties of Mixed-Matrix Membranes Via Combined Use of Two- and Three-Dimensional Fillers — **Tae-Hyun Bae**

**1:33 Paper 673d:** Enabling Molecular Sieving Behaviors of Mixed Matrix Membranes for Efficient  $\text{C}_3\text{H}_6/\text{C}_3\text{H}_8$  Separations — **Jong Suk Lee, Heseong An**

**1:54 Paper 673e:** Room-Temperature Synthesis of Functionalized Two-Dimensional Metal-Organic Frameworks for Enhanced  $\text{CO}_2/\text{CH}_4$  Separation — **Jie Zha, Xueyi Zhang**

**2:15 Paper 673f:** Adsorption-Enhanced, Plasticization Resistant Composite Membranes Using Metal-Organic Framework Nanocrystals — **Jonathan E. Bachman, Jeffrey R. Long**

**2:36 Paper 673g:** Synthesis of 2D MOF Nanosheets with Large Aspect Ratio through Control over Hydrogen Bond Formation for Membrane Separation — **Bohan Shan, Bin Mu, Sefaattin Tongay**

## (674) MOFs, COFs, and Porous Polymer Materials: Characterization and Application

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 329

Dongxia Liu, Co-Chair

**Sponsored by:** Inorganic Materials

**12:30 Paper 674a:** Negative Thermal Expansion Design Strategies in Metal-Organic Frameworks — **Nicholas C. Burtch**

**12:48 Paper 674b:** Towards a Generalized Understanding of the Acid Gas Stability of Zeolitic Imidazolate Frameworks (ZIFs) — **Souryadeep Bhattacharyya, Jayraj Joshi, Krista S. Walton, David S. Sholl, Sankar Nair**

**1:06 Paper 674c:** Controlling the Ion-Doping Mechanism in Defective UiO-66 — **Sean M. McIntyre, Bohan Shan, Bin Mu**

**1:24 Paper 674d:** Highly Selective, High-Capacity Metal-Organic Frameworks for Olefin Production — **Jonathan E. Bachman, Jeffrey R. Long**

**1:42 Paper 674e:** Stability of MOF Nanoparticles in High Ionic Strength Solutions — **Satish K. Nune, B. Peter McGrail**

**2:00 Paper 674f:** Ultrathin Covalent-Organic Framework Membranes for Organic Solvent Nanofiltration: A Molecular Simulation Study — **Wan Wei, Kang Zhang, Jianwen Jiang**

**2:18 Paper 674g:** Computational Screening of Metal-Organic Frameworks for Adsorption of Organophosphate Chemical Warfare Agents — **Mayank Agrawal, Jacob A. Harvey, Dorina F. Sava Gallis, Jeffery A. Greathouse, David S. Sholl**

**2:36 Paper 674h:** Novel Branched HKUST-1 Morphology for Improved Mixed Matrix Membrane Formation and Gas Separation Performance — **Daniel J. Harrigan, Benjamin J. Sundell, Ke Zhang, Steven C. Hayden, Won Seok Chi, Zachary Smith**

## (675) Multiscale Systems Biology

Thursday, Nov 1, 12:30 PM

Westin Convention Center, Butler

Ashlee N. Ford Versypt, Chair  
Steven M. Abel, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**12:30 Paper 675a:** Investigating Cellular Physiology of a Marine Cyanobacterium Using a Multi-Scale Multi-Paradigm Metabolic Model — **Joseph Gardner, Nanette R. Boyle, Bri-Mathias S. Hodge**

**12:48 Paper 675b:** Modeling, Optimization, and Control of Bioprocesses Using Optogenetics — **Robert J. Lovelett, Evan Zhao, Makoto A. Lalwani, Jared Toettcher, Ioannis G. Kevrekidis, Jose L. Avalos**

**1:06 Paper 675c:** Multiscale Modeling of Monoclonal Antibody (mAb) Production and Glycosylation in a Chinese Hamster Ovary (CHO) Cell Culture Process — **Yu Luo, J. Vincent Price, Robert J. Lovelett, Devesh Radhakrishnan, Kristopher Barnhouse, Eugene Schaefer, John Cunningham, Ping Hu, Kelvin H. Lee, Raghu Shivappa, Babatunde A. Ogunnaike**

**1:24 Paper 675d:** Mathematical Modeling of Metastatic Cancer Migration through a Remodeling Extracellular Matrix — **Yen T. Nguyen Edalgo, Ashlee N. Ford Versypt**

**1:42 Paper 675e:** A Multiscale Brownian Dynamics Model Predicts Diffusion-Controlled Multivalent Antigen-Receptor Assembly in the Cell Membrane — **Md Shahinuzzaman, Jawahar Khetan, Dipak Barua**

**2:00 Paper 675f:** Multiscale Prediction of Aggregation and Solubility of Amyloid-Derived Peptides — **Chris A. Kieslich**

**2:18 Paper 675g:** Invited Speaker: Systems Biology of Cancer – What Can We Learn? — **Aleksander Popel**

#### (676) Nanobiotechnology for Sensors and Imaging I

**Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 311

Daniel Roxbury, Chair

**Sponsored by:** Bionanotechnology

**12:30 Paper 676a:** Invited Talk: Towards In Vivo Bioimaging of Electrical Fields and Mechanical Forces with Stimuli-Responsive Upconverting Nanoparticles — **Jennifer Dionne, Randy Mehlenbacher, Alice Lay, Chris Siefe, Stefan Fischer**

**12:54 Paper 676b:** Development of Lspr-Based Biosensor for the Detection of Sjogren's Syndrome Biomarkers — **Andrew C. Murphy, Marissa E. Wechsler, John R. Clegg, Nicholas A. Peppas**

**1:12 Paper 676c:** Development of Protein-Gold Nanoparticle Based Colorimetric Radiation Sensor — **Amar Thaker, Brent L. Nannenga**

**1:30 Paper 676d:** Characterizing the Uptake of Quinic Acid and Tannic Acid Coated Iron Oxide Nanoparticles for Labeling of Cancer Cells — **Akshay Narkhede, Jennifer Sherwood, Kasie Coogan, Yuping Bao, Shreyas Rao**

**1:48 Paper 676e:** Tuneable Mechanical Response of Twisted DNA Nanotubes Towards Biosensing — **Sriram Kumar**

**2:06 Paper 676f:** Novel Fluorescent Nano Structures for Bio-Imaging of MCF-7 Cells — **Aishee Dey, Lopamudra Giri, Sudarsan Neogi**

**2:24 Paper 676g:** Engineered Green Fluorescent Proteins: Cartilage-Targeted Delivery Nanocarriers That Provide Insights on the Effects of Charge on Transport into Dense Charged Tissues — **Yamini Krishnan, Holly A. Rees, Christina P. Rossitto, Si-Eun Kim, Han-Hwa K. Hung, Eliot H. Frank, Bradley D. Olsen, David R. Liu, Paula T. Hammond, Alan Grodzinsky**

**2:42 Paper 676h:** Chemically Tuned NIR Light-Activated Bionanoparticles for the Selective Destruction of Tumor Cells in Heterocellular 3D Models and for Quantitative In Vivo tumor Imaging — **Girgis Obaid, Shazia Bano, Kimberly Samkoe, Srivallesha Mallidi, Jerrin Kuriakose, Brian Pogue, Tayyaba Hasan**

#### (677) New Technologies to Enhance the Production of Unconventional Oil and Natural Gas: Experimentation

**Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 321

Jared Ciferno, Chair  
Rameshwar D. Srivastava, Co-Chair  
Jason Trembly, Co-Chair  
David Cercone, Co-Chair

**Sponsored by:** Advances in Fossil Energy R&D

**12:30 Paper 677a:** New Technologies to Enhance the Production of Unconventional Oil and Natural Gas — **Jared Ciferno**

**12:52 Paper 677b:** Characterization of Microfractures in Organic-RICH Shales and Tight Reservoir Rocks of the Bakken Formation By Integrated Microscopy Techniques — **Alexander Azenkeng, Blaise Mibeck, Kurt Eylands, Shane Butler, Bethany Kurz**

**1:14 Paper 677c:** Remediation of Polyacrylamide-Induced Permeability Damage from Fracturing Using H<sub>2</sub>O<sub>2</sub> Catalyzed By Free and Immobilized Peroxidase Enzyme — **William J.R. Gilbert, Jyun Syung Tsau, Stephen J. Johnson, Jenn-Tai Liang, Aaron M. Scurto**

**1:36 Paper 677d:** Investigation of Scaling As a Means for Decreased Petroleum Production from the Utica/Point Pleasant Unconventional Play — **Michael Spencer, Jason Trembly, Ravinder Garlapalli**

**1:58 Paper 677e:** CO<sub>2</sub>-in-Mineral Oil Emulsions, CH<sub>4</sub>-in-Mineral Oil Foams and N<sub>2</sub>-in-Mineral Oil Foams Stabilized By Novel Oil-Soluble Surfactants As Waterless Hydraulic Fracturing Fluids — **Shehab Alzobaidi, Gianfranco Rodriguez, Jason J. Lee, Congwen Lu, Chang Da, Justin Harris, Robert J. Perry, Keith Johnston, Robert Enick**

**2:20 Paper 677f:** Hydraulic Fracture Propagation in Unconventional Reservoirs Under the Influence of Natural Fracture Heterogeneities — **Wei Fu, Alexei A. Savitski, Branko Damjanac, Andrew P. Bunker**

**2:42 Paper 677g:** Characterization of CO<sub>2</sub>, Fluid, and Shale Via Feature Relocation Using Field-Emission Scanning Electron Microscopy, in Situ Infrared Spectroscopy, and Pore Size Analysis — **Angela Goodman, Sean Sanguinito, Barbara Kutchko, Jeffery Culp, Sittichai Natesakhawat, Dustin Crandall**

#### (678) Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications I

**Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 413

Georgios A. Sotiriou, Chair  
Timothy Brenza, Co-Chair

**Sponsored by:** Nanoparticles

**12:30 Paper 678a:** Engineering the Surfaces of Fluorescently-Labeled Polymeric Nanoparticles for Drug Delivery — **Ami Jo, Rui Zhang, Judy Riffle, Ritchey M. Davis**

**12:50 Paper 678b:** Optimizing the Surface Property-Activity Relationship of Nanoscale Hydrogel Drug Delivery Systems — **Angela Wagner, Alex Shearer, Alexandria Lawrence, Bhaargavi Ashok, Nicholas A. Peppas**

**1:10 Paper 678c:** Paramagnetic Cations-Loaded Polydopamine Nanoparticles Cytotoxicity — **Milena Vega, Celia Nieto, Gema Marcelo, Miguel A. Galán, Eva Martín del Valle**

**1:30 Paper 678d:** Two-Photon Microscopy for Deep-Tissue Imaging of Dopaminergic Neuromodulation in the Brain — **Jackson Travis Del Bonis-O'Donnell, Ian McFarlane, Ralph Page, Abraham Beyene, Eric Tindall, Markita Landry**

**1:50 Paper 678e:** Ultrafast Post-Formulation Core Radiolabeling of Biodegradable Nanoparticles for PET Contrast Agents — **Leon Z. Wang, Tristan L. Lim, Prashanth Padakanti, Hoang D. Lu, Abass Alavi, Robert Mach, Robert K. Prud'homme**

**2:10 Paper 678f:** Voltage-Sensitive Ultrasound Enhancing Agent: *In Vitro* and *In Vivo* analysis — **Michael Cimorelli, Benjamin Andrien, Kyle Barrett, Aaron T. Fafarman, Andrew Kohut, Brett Angel, Steven P. Wrenn**

#### (679) Operation of Energy Systems

**Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 410

Fengqi You, Chair  
Mariano Martín, Co-Chair

**Sponsored by:** Computers in Operations and Information Processing

**12:30 Paper 679a:** The Impact of Microgrids on the Grid: Integration of Distributed Renewables Via Network-Constrained Affine Robust Unit Commitment — **Matthew J. Palys, Prodromos Daoutidis**

**12:49 Paper 679b:** Modeling and Optimization of Supercritical Pulverized Coal Power Plants Under Part Load Operation — **Jaffer Ghouse, John C. Eslick, Anthony P. Burgard, Andrew Lee, Miguel A. Zamarripa, Jinliang Ma, John P. Eason, Bethany Nicholson, Carl D. Laird, Lorenz T. Biegler, Debansu Bhattacharyya, David C. Miller**

**1:08 Paper 679c:** Cost-Effectiveness of Grid Energy Storage Technologies in Current and Future U.S. Power Systems — **Omar J. Guerra, Joshua Eichman, Bri-Mathias S. Hodge, Jennifer Kurtz**

**1:27 Paper 679d:** New Operating Strategy for a Combined Cycle Gas Turbine Power Plant — **Zuming Liu, Iftekhar A. Karimi**

**1:46 Paper 679e:** Flexible Carbon Capture Exploiting Dynamic Changes in Electricity Price — **Manali Zantye, M. M. Faruque Hasan**

**2:05 Paper 679f:** Stability-Preserving Economic Optimization of Microgrids — **Sungho Shin, Victor M. Zavala**

**2:24 Paper 679g:** Optimal Design of Aging Systems: A-Frame Coolers Design Under Fouling — **Jose A. Luceño, Mariano Martín**

**2:43 Paper 679h:** A Data-Driven Optimization Framework for Selection and Operation of Energy Storage Systems — **Lanyu Li, Tianxun Zhou, Xiaonan Wang**



**(680) Polymers for Energy Storage and Conversion****Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 327

Siamak Nejati, Chair  
Ying Diao, Co-Chair**Sponsored by:** Polymers**12:30 Paper 680a:** Aramid Nanofibers for Structural Enhancement of Capacitors and Batteries — *Se Ra Kwon, Evi Flouda, Anish Patel, James Boyd, Dimitris Lagoudas, Micah J. Green, Jodie L. Lutkenhaus***1:00 Paper 544hb:** Electrocatalytic Activity of Thin Polymeric Films Synthesized through Chemical Vapor Deposition — *Shayan Kaviani, Mahdi Mohammadi Ghaleni, Elham Tavakoli, Siamak Nejati***1:15 Paper 680c:** Polyethylene-Based Block Copolymer Alkaline Anion Exchange Membranes: Synthesis, Preparation, and Characterization — *Carrie L. Trant, Chulsung Bae, Sangwoo Lee***1:30 Paper 680d:** Single-Ion Conducting Polymer Membranes for Energy Storage Applications — *Pengfei Cao, Bingrui Li, Jagjit Nanda, Alexei Sokolov, Tomonori Saito***1:45 Paper 680e:** Ion Transport Properties of Ultra-Thin Film Polymer Electrolytes — *Ban Dong, Yu Kambe, Paul F. Nealey, Shrayesh N. Patel***2:00 Break****2:15 Paper 680g:** Ionic Liquid Imbibed Dual-Conducting Graphene-Polyacetylene Nanocomposite Membranes — *Aswin Prathap Pitchiya, Yanni Wang, Cody Johnson, Dipankar Roy, Sitaraman Krishnan***2:30 Paper 680h:** Biocompatible and Biodegradable Ionic Liquid Polymer Composite As Electrolyte for Implantable Energy Storage Device — *Vaishali Krishnadoss, Harrison Hawkins, Leah Filardi, Andrew Kapetanakis, Ethan Ellis, Nicole Rosselli, Jamie Shirtz, Tyler Hannah, Caleb Miller, Akshar Patel, Iman Noshadi***2:45 Paper 680i:** Comb Shaped Anion Conductive Ionomer Films for Electrochemical Energy Storage Devices — *Ananth Venkatachalam, Wayz R. Khan, Ashleigh Herrera, Christopher Cornelius***(681) Predictive Control and Optimization II****Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 408

Ravendra Singh, Chair  
Fernando V. Lima, Co-Chair**Sponsored by:** Systems and Process Control**12:30 Paper 681a:** Safe Economic Model Predictive Control of Nonlinear Systems — *Zhe Wu, Helen Durand, Panagiotis D. Christofides***12:49 Paper 681b:** Improving Flexibility and Energy Efficiency of a Post-Combustion CO<sub>2</sub> Capture Process Using Economic Model Predictive Control — *Benjamin Decardi-Nelson, Su Liu, Jinfeng Liu***1:08 Paper 681c:** Towards on-Line Development of Physically-Based Models for Model-Based Control Design — *Laura Giuliani, Helen Durand***1:27 Paper 681d:** Data Driven Economic Model Predictive Control for Unstable Systems — *Masoud Kheradmandi, Prashant Mhaskar***1:46 Paper 681e:** Incorporation of Sustainability and Economic Considerations in Process Control of Hydraulic Fracturing in Unconventional Reservoirs — *Priscille Etoughe, Prashanth Siddhamshetty, Kaiyu Cao, Rajib Mukherjee, Joseph Sangil Kwon***2:05 Paper 681f:** Multi-Objective Optimization of the Energy System in an Iron and Steel Plant Considering the Economic Cost and Life Cycle Environmental Impact — *Yujiao Zeng, Jie Li, Xin Xiao, Fei Song, Yaling Nie, Min Zhu***2:24 Paper 681g:** Model Predictive Control with Active Learning Under Model Uncertainty — *Tor Aksel N. Heirung, Ali Mesbah***2:43 Paper 681h:** A Modified SQP Method for MPC of a Supercritical Pulverized Coal-Fired Power Plant during Cycling — *Xin He, Fernando V. Lima***(682) Process Design: Innovation for Sustainability****Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 316

Yuan Yao, Chair  
Gerardo J. Ruiz-Mercado, Co-Chair  
Heriberto Cabezas, Co-Chair**Sponsored by:** General**12:30 Paper 682a:** Sustainable Ammonia Production through Process Synthesis and Optimization — *C. Doga Demirhan, William W. Tso, Joseph B. Powell, Efstratios N. Pistikopoulos***12:55 Paper 682b:** Modeling and Simulation of a Piston-Type Work Exchanger for Mechanical Energy Recovery — *Aida Amini Rankouhi, Yinlun Huang***1:20 Paper 682c:** Simulation-Based Computational Framework for Sustainability Assessment and Life Cycle Inventory Generation — *Shuyun Li, Selorme Agbleze, Gerardo J. Ruiz-Mercado, Fernando V. Lima***1:45 Paper 682d:** Designing Manufacturing Sites Toward Local Sustainability By Understanding Spatial Variance of Industrial Air Pollution and Local Ecosystem Regulation — *Michael Charles, Bhavik R. Bakshi***2:10 Paper 682e:** Sustainability Identification for N-Dimensional Systems — *Masih Jorat, Vasilios Manousiouthakis***2:35 Paper 682f:** Sustainability Assessment and Targeting in Process Design: A Novel Method Based on Data Envelopment Analysis - Application to Liquid Fuels — *Daniel F. Rodriguez-Vallejo, Ángel Galán Martín, Benoît Chachuat, Gonzalo Guillén-Gosálbez***(683) Software Engineering in and for the Molecular Sciences****Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 308

Eric Jankowski, Chair  
Heather J. Kulik, Co-Chair  
Heather Mayes, Co-Chair**Sponsored by:** Computational Molecular Science and Engineering Forum**12:30 Paper 683a:** Efficient Discovery of Novel Molecules: How to Uncover Gems in the Haystack — *Geoffrey Hutchison***1:00 Paper 683b:** Chemlg - a Smart and Massively Parallel Code to Accelerate the Molecular Library Generation — *Mohammad Atif Faiz Afzal, Johannes Hachmann***1:15 Paper 683c:** GOMC: GPU Optimized Monte Carlo for the Simulation of Phase Equilibria and Physical Properties of Complex Fluids. — *Mohammad Barhaghi, Younes Nejahi, Jason R. Mick, Brock Jackman, Kamel I. Rushaidat, Yanzhe Li, Loren Schwiebert, Jeffrey J. Potoff***1:30 Paper 683d:** Lancelot - an Open-Source Codebase for Simplified Computational Chemistry — *Henry C. Herbol, James Stevenson, Yaset Acevedo, Andrew Ruttinger, Paulette Clancy***1:45 Paper 683e:** Saffire: Enabling Large Scale Simulations of Rare Events — *Sapna Sarupria, Ryan DeFever, Walter Hanger, Linh Ngo, Amy Apon***2:15 Paper 683f:** Quantifying Nanostructure within Molecular Simulations Using Geometry-Based Criteria — *Michael L. Greenfield, Faramarz Joodaki***2:30 Paper 683g:** Runtime Code Generation for User-Configurable Metropolis Monte Carlo Energy Evaluation in HOOMD-Blue — *Joshua A. Anderson, William Zygmunt, Luis Y. Rivera-Rivera, Jens Glaser, Sharon C. Glotzer***2:45 Paper 683h:** Implementation of Harmonically Mapped Averaging Methods in Popular Molecular Simulation Codebases — *Apoorva Purohit, Sabry G. Moustafa, Arpit Bansal, Andrew J. Schultz, David A. Kofke***(684) Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond I****Thursday, Nov 1, 12:30 PM**

David L. Lawrence Convention Center, 302

Fang Wang, Chair  
Marina Tsiannou, Co-Chair  
Xiaobin Jiang, Co-Chair**Sponsored by:** Crystallization and Evaporation**12:30 Introductory Remarks****12:35 Paper 684a:** Polymorphic Selection of Biominerals By Anionic Polyelectrolytes — *Gopichand Mallam, Arkita Chakrabarti, Marina Tsiannou***12:55 Paper 684b:** Coupling Experimental Results with Molecular Dynamics Simulations to Describe Polymorphism Obtained Using Solution Shearing — *Stephanie Guthrie, Baoxing Xu, Yuan Gao, Gaurav Giri*

**1:15 Paper 684c:** Investigation of the Polymorphism Phenomenon of the Carotene Lutein — *Wei Guo, Shijie Xu, Shichao Du, Lina Jia, Yan Wang, Junbo Gong, Xiaoyue Tan*

**1:35 Paper 684d:** A Kinetic Study of Crystallization Process of Imatinib Mesylate with Polymorphic Transformation Phenomenon — *Mengxing Lin, Sohrab Rohani*

**1:55 Paper 684e:** Polymorphism of D-Mannitol: Selective Nucleation and Crystal Growth Mechanism — *Weiyi Su, Chunli Li, Honghai Wang, Jing Fang*

**2:15 Paper 684f:** Can the Solvation Manner Leads to a Nucleation Diversity for Polymorphic System? the Case of D-Mannitol — *Shiyuan Liu, Junbo Gong*

#### (685) Sustainability Metrics at the Process and Product Level Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 320

Larry Erickson, Chair  
Yinlun Huang, Co-Chair

**Sponsored by:** Sustainability

**12:30 Paper 685a:** Process and Supply Chain Design: Sustainability Metrics and Structural Considerations — *Heriberto Cabezas, Andres Argoti, Ferenc Friedler, Peter Mizsey, Jean Pimentel*

**12:55 Paper 685b:** Sustainability Assessment of Nanocoating Manufacturing — *Raha Gerami, Yinlun Huang*

**1:20 Paper 685c:** Comparative Life Cycle Assessment of Methanol Production Processes Based on Externalities Under Uncertainty — *Amjad Al-Qahtani, Andrea Bernardi, Andres Gonzalez, Gonzalo Guillén-Gosálbez,*

**1:45 Paper 685d:** Determining Chemical Release Profiles By Rapid Estimation Methods — *Raymond L. Smith, David E. Meyer, Gerardo J. Ruiz-Mercado, Michael A. Gonzalez, John P. Abraham, William M. Barrett*

**2:10 Paper 685e:** Design and Manufacture of a Torus Microreactor for the Removal of Azo Dyes By Laccase Immobilized on Magnetite Nanoparticles — *Mabel Juliana Noguera Contreras, Ana Lucía Campaña Perilla, Sergio Leonardo Flórez González, Christian Camilo Segura, Juan C Cruz, Johann F Osma*

**2:35 Paper 685f:** Gold Recovery from Electronic Waste By Nanoporous Polymers — *Yeongran Hong, Damien Thirion, Saravanan Subramanian, Cafer T. Yavuz*

#### (686) Water Treatment, Desalination, and Reuse I

Thursday, Nov 1, 12:30 PM

David L. Lawrence Convention Center, 304

Isabel Escobar, Co-Chair  
William A. Phillip, Co-Chair  
Mahdi Malmali, Co-Chair

**Sponsored by:** Membrane-Based Separations

**12:30 Paper 686a:** Bio-Inspired Immobilization of Casein-Coated Silver Nanoparticles on Cellulose Acetate Ultrafiltration Membranes for Biofouling Control — *Xiaobo Dong, Conor Sprick, Tequila Harris, Isabel Escobar*

**12:50 Paper 686b:** Concurrent Desalination and Boron Removal Via Reverse Osmosis — *Seda Kayaci, Sadiye Velioglu, Süer Kürklü, M. Goktug Ahunbay, S. Birgül Tantekin-Ersolmaz, William B. Krantz*

**1:10 Paper 686c:** Surface Nano-Structuring with Hydrophilic Polymer Brush Layers for Tailored Performance of Fouling Resistant RO and UF Membranes — *Soomin Kim, Yian Chen, Shangwen Zha, Anditya Rahardianto, Yoram Cohen*

**1:30 Paper 686d:** Dual-Functionalized Nanofiltration Membranes Exhibit Multifaceted Anti-Fouling and Ion Rejection Performance — *John R. Hoffman, Siyi Qu, Theodore Dilenschneider, Monica McFadden, William A. Phillip*

**1:50 Paper 686e:** Inorganic Microfiltration Membranes Modified with Hydrophilic Silica Nanoparticles for Oil-in-Water Emulsion Separation — *Ruochen Liu, Ashwin Kumar Yegya Raman, Imran Khan Shaik, Clint P. Aichele, Seok-Jhin Kim*

**2:10 Paper 686f:** Effect of the Surface Charge of Monodisperse Particulate Foulants on Cake Formation — *Qi Han, Thien An Trinh, Weiyei Li, Anthony G. Fane, Jia Wei Chew*

**2:30 Paper 686g:** Zwitterion-Substituted Polysulfones As Fouling-Resistant Desalination Membranes — *Matthew D. Green, Yi Yang*

#### (687) Adsorbent Materials: MOFs II

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 305

T. Grant Glover, Chair  
Bin Mu, Co-Chair

**Sponsored by:** Adsorption and Ion Exchange

**3:30 Paper 687a:** Probing Metal-Organic Framework (MOF) Design for Adsorptive Sour Natural Gas Purification — *Jayraj Joshi, Guanghui Zhu, Jason Lee, Eli Carter, Christopher W. Jones, Ryan Lively, Krista S. Walton*

**3:51 Paper 687b:** The Role of Solvent in the Room Temperature Synthesis of Two Isomeric Metal-Organic Frameworks — *Julian T. Hungerford, Krista S. Walton*

**4:12 Paper 687c:** Insight on Fluorinated MOFs Structural Properties-Gas/Vapor Adsorption/Sensing Relationships — *Youssef Belmabkhout, Mohamed Rachid Tchalala*

**4:33 Paper 687d:** Methane Adsorption on Zeolitic Imidazolate Framework-8 (ZIF-8) — *Dinuka H. Gallaba, Aldo Migone*

**4:54 Paper 687e:** Incorporation of a Dioxo-Molybdenum(VI) Complex into a Titanium-Functionalized Zr(IV)-Based Metal-Organic Framework — *César A. Bravo-Sanabria, Gustavo Ramírez-Caballero, Fernando Martínez-Ortega*

**5:15 Break**

**5:36 Paper 687g:** Moisture-Enhanced Feature for Potential CO<sub>2</sub> Capture Under Humid Conditions within Microporous PCN-250 Frameworks — *Qibin Xia, Yongwei Chen, Zhong Li*

#### (688) Advanced Structural Composites

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 329

Jiang Guo, Chair  
Jiahua Zhu, Co-Chair  
Jingjing Liu, Co-Chair

**Sponsored by:** Composites

**3:30 Paper 688a:** Thermally Conductive Scaffold for Leakage-Free Phase Change Materials — *Marjan Alsadat Kashfipour*

**3:48 Paper 688b:** Stress-Sensing Thermoset Polymer Networks Via Grafted Cinnamoyl Mechanophores in Epoxy — *Ryan Gunckel, Elizabeth M. Nofen, Bonsung Koo, Lenore L. Dai, Aditi Chattopadhyay*

**4:06 Paper 688c:** Analysis of Structure-Property Relationships Via Finite Element Method to Predict Composite Mechanical Properties and a Comparison of Homogenization Methods — *Joshua Arp, Mingzhe Jiang, Christopher L. Kitchens, Joseph Geddes, Sez Atamturktur, Andrew Brown*

**4:24 Paper 688d:** The Effect of Thermal Treatment on Electrospun Ceramic Nanofibers — *Oren Elishav, Vadim Beilin, Gennady E. Shter, Gideon S. Grader*

**4:42 Paper 688e:** Cure Monitoring of Glass-Fiber Reinforced Composite (GFRP) Laminates By in-Situ Strain Measurement — *Santoshi Mohanta, Swati Neogi*

**5:00 Paper 688f:** The Design of Advanced Non-Toxic Flame Retardants Based on DNA and DNA Functionalized Single-Walled Carbon Nanotubes — *Mohammad Moein Safaei, Daniel Roxbury*

**5:18 Paper 688g:** Exploiting Capillary Forces in Filled Plastics: Electrically Conductive Plastics By Bonding Copper Filler with Molten Solder — *Derrick Amoabeng, Sachin Velankar*

#### (689) Atomically Dispersed Supported Metal Catalysts II

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 406

Jean-Sabin McEwen, Chair  
Chao Wang, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 689a:** Characterization of Isolated Pt Atoms on Anatase TiO<sub>2</sub> — *Weiqing Zheng, Jiayi Fu, Jonathan Lym, Konstantinos Alexopoulos, Na Li, Jorge A. Boscoboinik, Dong Su, Dionisios G. Vlachos*

**3:51 Paper 689b:** The Marriage of Activity and Selectivity in the Oxidative and Non-Oxidative Activation of Methane on Gold-Palladium Alloys — *Quan Do, Hung-Vu Tran, Shengguang Wang, Lars C. Grabow*

**4:12 Paper 689c:** Periodic Trends in Adsorption Energies of Transition Metal Precursors on Reducible Cerium Oxide: Towards Rational Synthesis of Single-Site Catalysts — *Ahana Mukhopadhyay, Robert M. Rioux*

**4:33 Paper 689d:** Structure of the Highly Reduced CeO<sub>2</sub>{111} Surface and Its Interaction with Single Atom Rh — *George Xu Yan, Yu Tang, Franklin Tao, Philippe Sautet*

**4:54 Paper 689e:** Non-Oxidative Dehydrogenation of Ethanol to Acetaldehyde and Hydrogen on Nickel-Gold Single Atom Alloys — **Georgios Giannakakis, Antonios Trimpalis, Maria Flytzani-Stephanopoulos**

**5:15 Paper 689f:** Synthesis, Characterization and Reactivity of Heteroatom Single Site Pairs for Selective Ethylene Conversion — **Insoo Ro, Chithra Asokan, Phillip Christopher**

**5:36 Paper 689g:** Decoupling Individual Catalytic Behaviors of Cu Single Site, Dimer and Cluster over Ceria Surface — **Feng Ryan Wang**

#### (690) Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries II

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 325

Junyong Zhu, Chair  
Bo Hu, Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**3:30 Paper 690a:** Electricity Performance of Microbial Fuel Cell with Mixed Inoculation of Yeast and *E.coli* — **Jinxia Yuan, Shijie Liu**

**3:55 Break**

**4:20 Paper 690c:** Biological Detoxification of Lignocellulosic Biomass Hydrolysate Liquor for Enhanced Ethanol Production — **Bhanendra Singh, Saurav Datta**

**4:45 Paper 690d:** Minimizing Enzyme Inhibition through in-Situ Recyclable Ammonia Detoxification of the Whole Slurry Derived from Acid-Catalyzed Pretreatment of Lignocellulosic Biomass — **Rui Zhai, Kaiqiang Shi, Mingjie Jin**

**5:10 Paper 690e:** From Starch-Enriched Algal Biomass to Biobutanol Production – a Model-Based Optimisation Study — **Gonzalo M. Figueroa-Torres, Jon Pittman, Constantinos Theodoropoulos**

#### (691) Biomass Characterization, Pretreatment, and Fractionation II

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 324

Catherine E. Brewer, Chair  
Michael T. Timko, Co-Chair

**Sponsored by:** Biorefinery Technologies for Forest Based Lignocellulosic Biomass

**3:30 Paper 691a:** Evaluation of Structure, Topochemistry and Transport Reaction Processes in Plant Biomass during Pretreatment — **Sahana Ramanna, Bandaru V. Ramarao, Feng Xu, Shri Ramaswamy**

**3:50 Paper 691b:** Biomass Torrefaction in a Pulsed Fluidized Bed — **Ruixu Wang, Ziliang Wang, Xiaotao Bi, C. Jim Lim, Shahab Sokhansanj**

**4:10 Paper 691c:** Co-Hydrothermal Carbonization of Coal Refuse and Cow Manure Blend — **Shanta Mazumder, M. Toufiq Reza**

**4:30 Paper 691d:** Advanced Characterization of Poplar Variants for Understanding Plant Cell Wall Recalcitrance — **Samarthya Bhagia, Jaroslav Durkovic, Rastislav Lagana, Riddhi Shah, Chang Geun Yoo, Sai V. Pingali, Hugh O'Neill, Wellington Muchero, Gerald Tuskan, Brian H. Davison, Arthur J. Ragauskas**

**4:50 Paper 691e:** Simulation of CO<sub>2</sub> Gasification of Manure-Derived Hydrochar Using Aspen Plus — **Pretom Saha, M. Toufiq Reza**

**5:10 Paper 691f:** Biomass Residue Characterization for Their Potential Application As Biofuels — **Mudasir a Shah**

#### (692) Bioprinting of Scaffolds, Tissues, and Organs

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 328

Murat Guvendiren, Co-Chair  
Xiaoyang Xu, Co-Chair

**Sponsored by:** Biomaterials

**3:30 Paper 692a:** The Age of Application in Bioprinting — **Ricky Solorzano**

**3:48 Paper 692b:** Nanoengineered Ionic-Covalent Entanglement (NICE) Bioinks for 3D Bioprinting — **Akhilesh K. Gaharwar**

**4:06 Paper 692c:** Engineering a Highly Elastic Protein-Based Bioink for Printing Complex Soft Tissues — **Sohyung Lee, Andrew Spencer, Ehsan Shirzaei Sani, Nasim Annabi**

**4:24 Paper 692d:** Silk Protein-Based Hydrogels for 3D Printing of Tissue Constructs — **Julia A. Tumbic, Danielle L. Heichel, Kelly A. Burke**

**4:42 Paper 692e:** Bioprinting of Large-Scale Hydrogels with Build-in Vascular Channels — **Shen Ji, Emily Almeida, Murat Guvendiren**

**5:00 Paper 692f:** 3D Bio-Printed Model of Brain Tumor Microenvironment with Vascultures — **Vivian K. Lee, Hongyan Zou, Roland Friedel, Guohao Dai**

**5:18 Paper 692g:** A 3D Printed Microfluidic Bioreactor to Engineer Biphasic Construct — **Riccardo Gottardi, Giulio De Riccardis, Martina Avolio, Derek Nichols, Alessandro Piroso, Peter Alexander, Manuela Raimondi, Rocky Tuan**

**5:36 Paper 692h:** Photo-Crosslinked Chondroitin Sulfate a and Chitosan for Extruded Vascularization — **Sachith Vidanapathirana, Howard W. T. Matthew**

#### (693) Catalytic Biomass Conversion to Chemicals

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 323

Karthikeyan K. Ramasamy, Chair  
Olivier Baudouin, Co-Chair

**Sponsored by:** Alternate Fuels and New Technology

**3:30 Paper 693a:** Alcohols/ Mixed Oxygenates Conversion to Higher Ketones over Multifunctional Mixed Oxide Catalysts — **Senthil Subramaniam, Michel Gray, Mond Guo, Heather Job, Karthikeyan K. Ramasamy**

**3:50 Paper 693b:** Single-Step Co-Synthesis of Methanol, Dimethyl Ether and Dimethyl Carbonate from Biomass Derived Syngas — **Pramod Sripada, Anurag Parihar, Sankar Bhattacharya**

**4:10 Paper 693c:** Insight into the Reactions of Upgrading Bio Aldehydes to High Value Aromatic Precursors — **Kuan-Ting Lin, Mond Guo, Karthikeyan K. Ramasamy**

**4:30 Paper 693d:** A High Selective Catalyst for Hydrogenation of 2-Methylfuran to 2-Methyltetrahydrofuran — **Li Zengjie, Zhu Ming, Mei Hua**

**4:50 Paper 693e:** Glycerol-Free Biodiesel Production from Palm Oil and Supercritical Dimethyl/Diethyl Carbonate Mixtures with Trace Heterogeneous Base Catalyst — **Yixia Gao, Jiahui Gu, Zhong Xin**

**5:10 Paper 693f:** Process Simulation and Analysis to Study Yield Conversion of Vegetable Oil to Biodiesel — **Mayra A. Pantoja-Castro, Horacio González-Rodríguez, Luis Fernando García-Montaño, Carlos Antonio Márquez-Vera, Francisco López-Villarreal**

**5:30 Paper 693g:** Modelling a Process to Study Production Biofuels — **Mayra Agustina Pantoja-Castro, Francisco López-Villarreal, Carlos Antonio Márquez-Vera, Mario Moscosa-Santillán, Ozny Lydia Avilés Hernández**

**5:50 Paper 693h:** Lipase-Catalyzed Synthesis of Biodiesel from Insect Fat Using Methyl Acetate As an Acyl Acceptor — **Chinh Hoang Nguyen, Fu-Ming Wang, Chia-Hung Su**

#### (694) Catalytic Hydrocarbon Processing II: Non-Oxidative Upgrading of Light Hydrocarbons

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 403

Brandon O'Neill, Chair  
Prasanna Dasari, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 694a:** Selective C–H Bond Activation of Light Alkane Using Metal Phosphide Catalysts — **Jeonghyun Ko, William F. Schneider**

**3:50 Paper 694b:** Catalytic Upgrading of Olefins Under Methane Environment: Effect of Sulfur Poisons on Catalyst Performance and Reusability — **Jonathan Harry, Aiguo Wang, Peng He, Hua Song**

**4:10 Paper 694c:** MOF-Derived Catalysts for Propane Dehydrogenation — **Michele L. Sarazen, Christopher W. Jones**

**4:30 Paper 694d:** DFT Investigation of the Mechanism and Site Requirements for Alkane Dehydrogenation on Transition Metal Sulfide Catalysts — **Ronak Upadhyay, Lohit Sharma, Jonas Baltrusaitis, Srinivas Rangarajan**

**4:50 Paper 694e:** The Migration of Pt and Its Application in the Activation of C–H Bonds of Ethane — **Junjun Shan, Hui Wang, Lisa Nguyen, John Matsubu, Yizhi Xiang, Fu-Kuo Chiang, Jihong Cheng**

**5:10 Paper 694f:** Co-Oligomerization of Ethylene and Propylene on Acidic Zeolites: A Microkinetic Model — **Sergio Vernuccio, Linda J. Broadbelt**



**5:30 Paper 694g:** Transient Kinetics Analysis of Ethane Aromatization over Metal Functionalized ZSM-5 Catalyst — *Yizhi Xiang, Tingyu Liang, Hossein Toghiani*

**(695) Catalytic Processing of Fossil and Biorenewable Feedstocks II: Upgrading Bio-Oils & Lignin**  
**Thursday, Nov 1, 3:30 PM**  
 David L. Lawrence Convention Center, 405

George Tsilomelekis, Chair  
 Jeremy S. Luterbacher, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 695a:** Gas Phase Catalytic Oxidation of Lignin to Produce Phenolic Compounds over Vanadia Catalysts — *Matthew M. Yung, Calvin Mukarakate, Mark Nimlos, Michael B. Griffin, Seonah Kim, Eric C. D. Tan*

**3:48 Paper 695b:** Mechanistic Study of the Hydrogenolysis of Diaryl Ethers Catalyzed By Heterogeneous Metal Catalysts — *Meng Wang, Oliver Gutiérrez, Donald M. Camaioni, Johannes A. Lercher*

**4:06 Paper 695c:** Palladium-Iron Bimetallic Catalyst: High Activity and Stability for Aqueous Phase Hydrogenations — *Yan Cheng, Hien N. Pham, Robert L. Johnson, Brent H. Shanks, Abhaya K. Datye*

**4:24 Paper 695d:** Hydrodeoxygenation of Guaiacol over Ni and Mo Nanoparticles Supported on SBA-15 and  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>. — *Thiago L. R. Hewer, Rubens W.S. Lima, Reinaldo Giudici, Martin Schmal, Rita M. B. Alves*

**4:42 Paper 695e:** Hydroprocessing of Biomass-Derived Oxygenates on Metal-Exchanged Zeolites Using Light Alkanes As the Source of Hydrogen — *Dante Simonetti, Eric Lin*

**5:00 Paper 695f:** Flowthrough Reductive Catalytic Fractionation of Biomass — *Eric Anderson, Michael Stone, Rui Katahira, Michelle Reed, Gregg T. Beckham, Yuriy Román-Leshkov*

**5:18 Break**

**5:36 Paper 695h:** Hydrodeoxygenation of Sorbitol to Monofunctional Fuel Precursors over Co/TiO<sub>2</sub> — *Nathaniel Eagan, Joseph P. Chada, Ashley Wittrig, J. Scott Buchanan, George W. Huber, James A. Dumesic*

**(696) Computational Methods in Biological and Biomedical Systems**  
**Thursday, Nov 1, 3:30 PM**  
 David L. Lawrence Convention Center, 408

Roman Voronov, Chair  
 Nigel Reuel, Co-Chair  
 Stacey D. Finley, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

**3:30 Paper 696a:** A Model-Based Algorithm for Subtyping Patients with Clotting Abnormalities Using Thromboelastogram Response — *Michelle Pressly, Matthew Neal, Gilles Clermont, Robert S. Parker*

**3:49 Paper 696b:** Hemolysis Prediction from CFD Simulations of Turbulent Blood Flow in a Functioning and Malfunctioning Bi-Leaflet Artificial Heart Valve — *Madison James, Edgar A. O'Rear, Dimitrios V. Papavassiliou*

**4:08 Paper 696c:** Dynamic Modeling of Cardiovascular System for Optimal Control of Ventricular Assist Devices — *Jeongeun Son, Yuncheng Du*

**4:27 Paper 696d:** First Passage of Molecular Motors on Networks of Cytoskeletal Filaments — *Paul J. Mlynarczyk, Steven M. Abel*

**4:46 Paper 696f:** Numerical Accuracy Comparison of Boundary Conditions Commonly Used for Approximating Shear Stress Distributions in Tissue Engineering Scaffolds Cultured Under Perfusion — *Olufemi Kadri, Cortes Williams III, Vassilios I. Sikavitsas, Roman Voronov*

**5:05 Paper 696g:** An *in-Silico* study of Feedforward Predictive Control in Blood Glucose Concentration for People with Type 1 Diabetes — *Yong Mei, Derrick Rollins*

**5:24 Paper 696h:** A Model-Based Investigation of Cytokine Storm for T-Cell Therapy — *Boorks Hopkins, Matthew Tucker, Yiming Pan, Zuyi (Jacky) Huang*

**5:43 Paper 696e:** Data-Driven Discovery of Novel Therapeutic Targets through Metabolic Modeling of *Staphylococcus Aureus* — *Mohammad Mazharul Islam, Vinai Chittozhram Thomas, Rajib Saha*

**(697) Control Strategy Development for Continuous Drug Substance and Drug Product Manufacture**  
**Thursday, Nov 1, 3:30 PM**  
 Westin Convention Center, Somerset

James C. Marek, Chair  
 Nima Yazdanpanah, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 697a:** Process Modelling, Simulation and Optimisation for Continuous Biopharmaceutical Manufacturing — *Samir Diab, Haruku Shirahata, Hirokazu Sugiyama, Dimitrios I. Gerogiorgis*

**3:50 Paper 697b:** Process Control Strategies for Pharmaceutical Drug Product Continuous Manufacturing – Where Are We Now and Where Do We Go from Here? — *Ian Leavesley*

**4:10 Paper 697c:** Data Accuracy for Smart Manufacturing in Continuous Pharmaceutical Systems — *Sudarshan Ganesh, Mariana Moreno, Qinglin Su, Yash Shah, Zoltan K. Nagy, G. V. Rex Reklaitis*

**4:30 Paper 697d:** Impurity Control in the Continuous Reactive Crystallization of Beta-Lactam Antibiotics — *Matthew A. McDonald, Andreas S. Bommarius, Ronald W. Rousseau, Martha A. Grover*

**4:50 Paper 697e:** Continuous Processing of Complex Dosage Forms: Liposomes and Polymeric Micelles — *Antonio Costa, Raj Mukherjee, Anand Gupta, Gowtham Yenduri, Xiaoming Xu, Celia N. Cruz, Bodhisattwa Chaudhuri, Diane Burgess*

**5:10 Paper 697f:** Active Process Control in the Quality-By-Design (QbD) Implementation of Pharmaceutical Continuous Tablet Manufacturing — *Qinglin Su, Yasasvi Bommireddy, Sudarshan Ganesh, Marcial Gonzalez, Gintaras V. Reklaitis, Zoltan K. Nagy*

**5:30 Paper 697g:** Modelling and Control of Continuous Wet Granulation in Co-Rotating Twin Screw Using Process Analytical Tools (PAT) — *Hamza Ismail, Darren Whitaker, Ahmad Albadarin, Mehakpreet Singh, Gavin Walker*

**(698) CO<sub>2</sub> Industrial, Engineering and R&D Approaches**  
**Thursday, Nov 1, 3:30 PM**  
 David L. Lawrence Convention Center, 320

Kevin C. Leonard, Chair

**Sponsored by:** Sustainability

**3:30** Introductory Remarks

**3:35 Paper 698a:** Green CO<sub>2</sub> Capture and Thorough Conversion: Two-Step Accelerated Mineral Carbonation and Simultaneously the Potential Combination with Seawater Softening — *Yingying Zhao, Mengfan Wu, Junsheng Yuan*

**3:53 Paper 698b:** Economic Assessment of Novel Process Turning Industrial Waste Gases (mixed CO/CO<sub>2</sub> streams) into Intermediates for Polyurethanes for Rigid Foams and Coatings — *Jason Collis*

**4:11 Paper 698c:** Techno-Economic Assessment of CO<sub>2</sub> and SO<sub>x</sub> Capture Process By Dilute Aqueous Ammonia — *Hoan Le Quoc Nguyen, David Shan-Hill Wong*

**4:29 Paper 698d:** World's Largest Commercial CO<sub>2</sub> to Methanol Demonstration Plant — *Christiaan Richter, Dana Marlin, Carlos Atli Córdova Geirdal*

**4:47 Break**

**4:57 Paper 698e:** Electrochemical CO<sub>2</sub> Conversion — *Charles Shanaughnessy, Kevin C. Leonard*

**5:15 Paper 698f:** Direct Carbonation of Ca(OH)<sub>2</sub> Using Super Critical CO<sub>2</sub> at Different Temperatures Along with the Introduction of SiO<sub>2</sub> Aggregate — *Daniel Klingenberg, Joseph J. Biernacki*

**5:33 Paper 698g:** Catalytic CO<sub>2</sub> Desorption in CO<sub>2</sub>-Loaded Aqueous MEA Solution over SO<sub>4</sub><sup>2-</sup>/ZrO<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub> Catalysts — *Xiaowen Zhang, Helei Liu, Jieliang Hong, Paitoon Tontiwachwuthikul, Zhiwu Liang*

**5:51 Paper 698h:** Carboxylation of Propylene Oxide to Propylene Carbonate — *Pallavi Bobba, Raghunath V. Chaudhari*

**6:09** Concluding Remarks

## (699) Data Science in Catalysis II

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 402

Zachary Ulissi, Chair  
Andrew Medford, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 699a:** Catkit: Symmetry Methods for Automated Generation of Catalytic Structures — **Jacob R. Boes**, Thomas Bligaard

**3:50 Paper 699b:** Predicting Adsorption Properties on Bimetallic Alloys As a Function of Local Morphology and Atomic Composition — **Tej S. Choksi**, Luke Roling, Frank Abild-Pedersen

**4:10 Paper 699c:** Insights from Machine Learning on a Large Database of Adsorption Energies — **Matthew M. Montemore**, Robert Hoyt, Ioanna Fampiou, Wei Chen, Tess Smidt, Kai Kohlhoff, Patrick Riley, Efthimios Kaxiras

**4:30 Paper 699d:** Methods to Exploit Large Datasets in Catalysis — **Kevin Tran**, Zachary Ulissi

**4:50 Paper 699e:** Generalized Geometric Descriptors for Oxygen Reduction Activity on Transition Metal Sulfides — **Dilip Krishnamurthy**, Venkatasubramanian Viswanathan

**5:10 Paper 699f:** Quantifying Confidence in DFT Predicted Surface Pourbaix Diagrams at Solid-Liquid Interfaces on Transition Metal Surfaces — **Olga Vinogradova**, Dilip Krishnamurthy, Vikram Pande, Venkatasubramanian Viswanathan

**5:30 Paper 699g:** Accelerating Inorganic Discovery with Machine Learning and Automation — **Heather J. Kulik**, Jon Paul Janet, Aditya Nandy, Chenru Duan, Stefan Gugler

## (700) Design and Operations Under Uncertainty II

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 410

Vijay Gupta, Co-Chair  
Qi Zhang, Co-Chair

**Sponsored by:** Systems and Process Design

**3:30 Paper 700a:** A Process Resilience Analysis Framework (PRAF) Application for Recoverability Assessment Model of Offshore Oil and Gas Platforms — **Purna Jain**, Efstratios N. Pistikopoulos, M. Sam Mannan

**3:49 Paper 700b:** A Mixed-Integer Programming Framework for Combined Placement of Fire and Gas Detectors in Chemical Processing Facilities — **Todd Zhen**, Katherine A. Klise, Bethany Nicholson, Carl D. Laird

**4:08 Paper 700c:** Optimal Design, Control and Scheduling of Multi-Product Systems Under Uncertainty: A Stochastic Back-Off Approach — **Robert Koller**, **Luis A. Ricardez-Sandoval**, Lorenz T. Biegler

**4:27 Paper 700d:** Risk-Averse Health-Aware Control of Subsea Plants — **Adriaen Verheyleweghen**, Johannes Jäschke

**4:46 Paper 700e:** Analytical and Triangular Representation of Flexibility Space — **Fei Zhao**, **Xi Chen**

**5:05 Paper 700f:** Design of Flare Systems Under Uncertainty: A Chance-Constrained Nonlinear Programming Approach — **Javier Tovar-Facio**, José M. Ponce, Yankai Cao, Victor M. Zavala

**5:24 Paper 700g:** Multistage Stochastic Programming Using Hybrid Scenario and Decision Rule Formulation — **Farough Motamed Nasab**, **Zukui Li**

**5:43 Paper 700h:** Optimization of Wastewater Treatment Plant Design Using an Early-Stage Techno-Economic Analysis Under Uncertainty — **Resul AI**, Chitta Ranjan Behera, Alexandr Zubov, Krist V. Gernaey, Gürkan Sin

## (701) Electrochemistry for Applications in Sustainability

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 306

Lauren F. Greenlee, Chair  
Gang Wu, Co-Chair  
Nian Liu, Co-Chair

**Sponsored by:** Electrochemical Fundamentals

**3:30 Paper 701a:** Tailoring Electrocatalytic Surfaces for Selective Alcohol Functionalization (*Invited*) — **Karthish Manthiram**

**3:50 Paper 701b:** Advanced Electrocatalysts for CO<sub>2</sub> and O<sub>2</sub> Reduction (*Invited*) — **Chao Wang**

**4:10 Paper 701c:** Evaluating the Economic Feasibility of Valorizing Lignocellulosic Biomass through Electrochemical Hydrogenation (*Invited*) — **Michael Orella**, Yuriy Román-Leshkov, **Fikile Brushett**

**4:30 Paper 701d:** Co-Electrolysis to Achieve Energy Efficient and Economic Conversion of CO<sub>2</sub> into Intermediates Such As CO and Ethylene (*Invited*) — **Paul J.A. Kenis**

**4:50 Paper 701e:** Electrocatalytic Interface Engineering with Ionic Liquids — **Joshua Snyder**, Yawei Li

**5:10 Paper 701f:** Design of Non-Stoichiometric Mixed Metal Oxides Toward the Advancement of Intermediate Temperature Solid Oxide Fuel Cells — **Juliana S. A. Carneiro**, Xiang-Kui Gu, Eranda Nikolla

**5:30 Paper 701g:** Pt Nanoparticles on Sb-SnO<sub>2</sub> Is an Ultra-Stable, Active Oxygen Reduction Reaction (ORR) Catalyst — **Cheng He**, Andrew Ells, Shrihari Sankarasubramanian, Vijay Ramani

**5:50 Paper 701h:** Electrocatalysts for Oxygen Reactions — **Hong Yang**

## (702) Engineering in Cancer Biology and Therapy II: Tumor Microenvironment and Mechanics

Thursday, Nov 1, 3:30 PM

Westin Convention Center, Cambria

Matthew Paszek, Co-Chair  
Marjan Rafat, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**3:30 Paper 702a:** Characterizing Interstitial Fluid Flow and the Effects of Shear Stress in the Brain Tumor Microenvironment — **R. Chase Cornelison**, Kathryn M. Kingsmore, Caroline E. Brennan, Steven Tom, Jennifer M. Munson

**3:48 Paper 702b:** Tissue Architectural Cues and Differential Extravasation Patterns Drive the Non-Random Trafficking of Tumor Cells in Larval Zebrafish — **Colin D. Paul**, Kevin Bishop, Alexis Devine, William J. Wulftange, Elliott L. Paine, Jack R. Staunton, Steven Shema, Val Bliskovsky, Lisa M. Miller Jenkins, Nicole Y. Morgan, Raman Sood, Kandice Tanner

**4:06 Paper 702c:** Perinuclear Actin Flow Promotes Efficient Cell Migration in Confinement — **Panagiotis Mistrionis**, Emily Wisniewski, Yizeng Li, Robert Law, Kaustav Bera, Soontorn Tuntithavornwat, Alexandros Athinios, Runchen Zhao, Sean X. Sun, Petr Kalab, Konstantinos Konstantopoulos

**4:24 Paper 702d:** Enhanced Capture and Release of Circulating Tumor Cells Using Hollow Glass Microspheres with Nanostructured Surface — **Ziye Dong**, Dan Yu, Wei Li

**4:42 Paper 702e:** A Cell-Friendly 3D Culture System for Scalable Culturing of Primary Human Glioblastoma Tumor-Initiating Cells — **Qiang Li**, Haishuang Lin, Ou Wang, Yuguo Lei

**3:30 Paper 702f:** Computational Study of Microscopic Drug Transport and Distribution in Tumor Vasculature — **Moath Alamer**, Xiao Yun Xu

**5:18 Paper 702g:** Invited Speaker: Engineering Microenvironments for Probing and Manipulating Cellular Mechanical Activities — **Yu-li Wang**

## (703) Fluid Particle Separation in Industrial and Environmental Systems

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 301

Isaac Gamwo, Chair  
Solmaz Tabatabaei, Co-Chair

**Sponsored by:** Fluid-Particle Separations

**3:30 Paper 703a:** Advanced Froth Flotation Using Oil-Coated Bubbles and Its Application in De-Inking — **Songcheng Wang**, Xiaotang Du, J. Carson Meredith, Sven H. Behrens

**3:55 Paper 703b:** Tribo-Charging of Binary Mixtures Composed of Coarse and Fine Particles in Gas-Solid Pipe Flow — **Haifeng Wang**, **Farzam Fotovat**, Xiaotao T. Bi, John R. Grace

**4:20 Paper 703c:** Simultaneous Separation of Protein and Starch Particles in Oat Flour Via Dry Fractionation Approaches — **Solmaz Tabatabaei**, Dinara Konakbayeva

**4:45 Paper 703d:** Investigation of *Shewanella Oneidensis* MR-1 and Community 31 for Microbial Reduction of Iodate at the Hanford Site — **Tafadzwa Chigumira**, Deondre Glover, Ayomikun Olarinoye, Patrick Ymeleleki, Yaolin Fennell, Kimberly L. Jones

**5:10 Paper 703e:** Application of a Hydrocyclone for Sludge Processing in a Wastewater Treatment Plant — **Thomas Senfter**, Martin Pillei, Manuel Berger, Roland Eisendle, Anke Bockreis, Wolfgang Rauch, Michael Kraxner

**(704) Fundamentals of Catalysis III: Oxidation in Supported Catalysis****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 401

Thomas J. Schwartz, Chair  
Konstantinos A. Goulas, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**3:30 Paper 704a:** Mechanistic Insights into the Direct Propylene Epoxidation over Au/TiO<sub>2</sub>/SiO<sub>2</sub> — **Jingjing Ji, Zheng Lu, Yu Lei, C. Heath Turner****3:48 Paper 704b:** Effect of PdCu Alloy Composition on Reactivity and Selectivity for Ethylene Acetoxidation to Vinyl Acetate — **Zhaoru Zha, Annamalai Leelavathi, Prashant Deshlahra****4:06 Paper 704c:** Kinetics of Ethylene Oxidation As a Function of Chlorine Coverage over a Highly-Promoted Ag/α-Al<sub>2</sub>O<sub>3</sub> Catalyst — **James W. Harris, Cha-Jung (Maria) Chen, Aditya Bhan****4:24 Paper 704d:** Kinetics of the Oxidative Cleavage of Methyl Ketones over Supported Vanadium Oxide Catalysts — **Ran Zhu, Siwen Wang, Jesse Q. Bond****4:42 Paper 704e:** Low-Temperature Selective Oxidation of Methanol to Formaldehyde over Pt-Bi Bimetallic Catalysts — **Yang Xiao, Yuan Wang, Arvind Varma****5:00 Paper 704f:** Water As Poison for H<sub>2</sub> Activation Sites at Au/TiO<sub>2</sub> Interface: Implications for Prox of H<sub>2</sub> in Water-Gas Shift Streams — **Sravan Kumar Kanchari Bavajigari, Todd Whittaker, Bert D. Chandler, Lars C. Grabow****5:18 Paper 704g:** Influence of Support and Environment on the Structure and Properties of Oxide Supported Isolated Pt Atoms — **Joaquin Resasco, Leo DeRita, Phillip Christopher****5:36 Paper 704h:** Effect of Dopants on the Activity and Selectivity in the Oxidative Coupling of Methane over Rare Earth Oxides — **Andrew S Jones, Helena E. Hagelin-Weaver****(705) Fundamentals of Sustainability Science and Engineering****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 319

Heriberto Cabezas, Chair  
Bhavik R. Bakshi, Co-Chair**Sponsored by:** Fundamentals**3:30 Paper 705a:** Optimization of Sustainable Processes Incorporating Data Envelopment Analysis — **Andres Gonzalez-Garay, Gonzalo Guillén-Gosálbez,****3:55 Paper 705b:** A Novel Model Predictive Control Scheme for Sustainability: Application to Biomass/Coal Co-Gasification System — **Shuyun Li, Gerardo J. Ruiz-Mercado, Fernando V. Lima****4:20 Paper 705c:** Sustainability Dynamics and Control for Distributed Manufacturing of Renewable Energy — **Raha Gerami, Majid Moradi Aliabadi, Yinlun Huang****4:45 Paper 705d:** An Analysis of Socioeconomic Impacts of Aviation Biofuel Development in Brazil — **Zhizhen Wang, Farahnaz Pashaei Kamali, Patricia Osseweijer, John A. Posada****5:10 Paper 705e:** A Coordinated Multi-Product Market for Organic Waste Management — **Yicheng Hu, Apoorva Sampat, Gerardo J. Ruiz-Mercado, Victor M. Zavala****5:35 Paper 705f:** Vulnerability of United States Industrial Sectors Dependent on Insect-Mediated Pollination Service — **Alex Jordan, Margaret Douglas, Harland Patch, Christina Grozinger, Vikas Khanna****(706) Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion II****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 310

Megan A. Creighton, Chair  
Carlos Silvera Batista, Co-Chair  
Evan K. Wujcik, Co-Chair**Sponsored by:** Carbon Nanomaterials**3:30 Paper 706a:** Effects of Pore Morphology and Pore Edge Termination on the Mechanical Behavior of Graphene Nanomeshes — **Mengxi Chen, Lin Hu, Ashwin Ramasubramaniam, Dimitrios Maroudas****3:50 Paper 706b:** Influence of Sonication Conditions and Wrapping Type on Yield and Fluorescent Quality of Noncovalently Functionalized Single-Walled Carbon Nanotubes — **Nathaniel Kallmyer, Trinh Huynh, Joseph Connor Graves, Joseph Musielewicz, Nigel Reuel****4:10 Paper 706c:** DNA-Controlled Brightening of Carbon Nanotube Photoluminescence in Acidic Environments — **Geyou Ao, Niyousha Mohammadshafie****4:30 Paper 706d:** Study on the Interfacial Interaction between Carbon Nanotubes and Catalyst: The Effects on the Tube Diameter — **Mauricio Carvajal Diaz, Perla B. Balbuena****4:50 Paper 706e:** Ionic Strength-Mediated Phase Transitions of Surface-Adsorbed DNA on Single-Walled Carbon Nanotubes — **Daniel P. Salem, Xun Gong, Albert Tianxiang Liu, Volodymyr Koman, Juyao Dong, Michael Strano****5:10 Paper 706f:** Graphene Oxide Model Development Via Reactive Molecular Dynamics Simulations — **Qi Qiao, Liangliang Huang****5:30 Paper 706g:** Analysis of Surfactant Exchange Kinetics of DNA-Wrapped Carbon Nanotubes — **Niyousha Mohammadshafie, Fjorela Xhyliu, Geyou Ao****(707) Highlights from the 20th Symposium on Thermophysical Properties (Invited Talks)****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 307

Paul M. Mathias, Chair  
Kenneth Kroenlein, Co-Chair**Sponsored by:** Thermodynamics and Transport Properties**3:30** Introductory Remarks**3:35 Paper 707a:** Application of Nuclear Magnetic Resonance Spectroscopy for the *in-Situ* Measurement of Vapor-Liquid Equilibria of Fluid Mixtures — **Christopher Suiter, Jason A. Widegren, Mark O. McLinden****4:04 Paper 707b:** Developing of a Universal Activity Correlation for Strong Electrolyte Systems — **Amadeu Sum, Shiang-Tai Lin****4:33 Paper 707c:** Molecular Dynamics Simulations of NMR Relaxation: Concepts and Applications to Hydrocarbons and Water in Confined Systems — **Dilip Asthagiri, Arjun V. Parambathu, Philip Singer, George J. Hirasaki, Walter G. Chapman****5:02 Paper 707d:** Reference Correlations for the Thermal Conductivity of Selected Molten Salts — **Chryssa Chliatzou, Marc Assael, Marcia Huber, William Wakeham****5:31 Paper 707e:** Impact of "Rough" Hydrate Particles in Slurry Rheology Modelling — **Zachary Aman, Yahua Qin, Paul Pickering, Eric F. May, Michael L. Johns****(708) Inhomogeneous Polymers****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 331

Matthew D. Green, Chair  
Ian Hosein, Co-Chair**Sponsored by:** Polymers**3:30 Paper 708a:** Using Crystallization to Control Filler Dispersion in Polymer Nanocomposites — **Sanat K. Kumar****4:00 Paper 708b:** Crystallization-Induced Stress Generation in Crosslinked Elastomers — **Jeh-Chang Yang, Xin Huang, Yuan Meng, Mitchell Anthamatten****4:15 Paper 708c:** Heterogeneous Morphologies, Crystallization Behaviors, Rheological and Thermo-Mechanical Properties of Thermoplastic Polyolefins of Ipp and Obc Blends — **Aizezi Maimaitiming, Guozhong Wu****4:30 Paper 708d:** A Universal Scaling Law for Block Copolymer Feature Sizes — **Amy Goodson, Julie N. L. Albert, Henry S. Ashbaugh****4:45 Paper 708e:** Hierarchical Assembly of Inhomogeneous Supramolecular Polymers from Hybrid Particle-Field Simulations — **Dong Meng, Jing Zong****5:00 Paper 708f:** Porous Thin Films with Hierarchical Structures Formed By Self-Assembly of Zwitterionic Comb Copolymers — **Ayşe Asatekin, Papatya Kaner, Ilcin Sadeghi****5:15 Paper 708g:** Symmetric Addition of Homopolymer on Ler/Lwr in Lamellae-Forming Directed Self-Assembled Block Copolymers — **Caleb Breaux, Jakin B. Delony, Peter Ludovice, Clifford L. Henderson****5:30 Paper 708h:** Understanding Failure Behavior of a Physically Assembled Thermoreversible Triblock Copolymer Gel — **Satish Mishra, Thomas E. Lacy, Santanu Kundu**Information as of  
September 25, 2018.  
An up-to-date program is  
available at [aiche.org/annual](http://aiche.org/annual)  
or on the AICHEvents app.



**5:45 Paper 708i:** Reduction in d-Spacing and Volume of Microphase Separated Acrylate Block Copolymers during Casting from Solution — **Alicia R. Pape, Rui Zhang, Louis Madsen, John A. Pople, Stephen M. Martin**

#### **(709) Interfacial Phenomena in Ionic Liquids**

**Thursday, Nov 1, 3:30 PM**  
Omni William Penn Hotel, Conference Center B

Younjin Min, Chair  
Lei Li, Co-Chair  
Paschalis Alexandridis, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 709a:** Enhancement of Self-Diffusion of Ionic Liquids Near Electrodes By an Electric Field — **Phwey Gil, Sara J. Jorgenson, Adriaan Riet, Burcu Gurkan, Daniel J. Lacks**

**3:45 Paper 709b:** Novel Hybrid Electrode-Electrolyte Materials Based on Ionic Liquids and Reduced Graphene Oxide for Supercapacitors — **Qianwen Huang, Qinmo Luo, Peiran Wei, Emily Pentzer, Burcu Gurkan**

**4:00 Paper 709c:** Visualizing Sorption and Anomalous Solute Diffusion in Ionic Liquids and Ionogels — **Alexandra V. Bayles, Matthew E. Helgeson, Todd M. Squires**

**4:15 Paper 709d:** Optimization of Ionic Liquid-Salt Aqueous Two-Phase System for Enzymatic Saccharification of Cellulose — **Kazuhiro Tanimura, Keishi Suga, Makoto Yoshimoto, Yukihiko Okamoto, Hiroshi Umakoshi**

**4:30 Paper 709e:** The Molecular Structure of Ionic Liquids at the IL/Solid Interface: Uncovering the Effect of Water — **Bingchen Wang, Lei Li**

**4:45 Paper 709f:** Solvation of Ionic Liquids on Supercapacitor's Performance: Insights from Molecular Dynamics Simulation — **Yu Zhang, Peter T. Cummings**

**5:00 Paper 709g:** Understanding Cellulose Solubility in Quaternary Onium Salt/Water/Urea Mixtures — **Mikayla Walters, Christy Wheeler West, Brooks D. Rabideau**

**5:15 Paper 709h:** Low Concentration of Ionic Liquids in Glycol Ether: Interfacial Layering Friction Behavior — **Rong An, Liangliang Huang, Faiz Ullah Shah**

#### **(710) Making Molecular Simulation a Mainstream Chemical Engineering Tool**

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 308

Michael R. Shirts, Chair  
Heather Mayes, Co-Chair

**Sponsored by:** Computational Molecular Science and Engineering Forum

**3:30 Paper 710a:** The Living Journal of Computational Molecular Science: Improving Community Use of Molecular Simulation Methods through a New Publishing Model — **Michael R. Shirts, David L. Mobley, Daniel M. Zuckerman**

**3:40 Paper 710b:** Strategies and Software for Accelerating Inorganic Molecular Design — **Heather J. Kulik, Jon Paul Janet, Chenru Duan, Aditya Nandy, Stefan Gugler**

**3:55 Paper 710c:** Computational Materials Education and Training (COMET): A Graduate Training Program to Teach Fundamentals of Quantum Density Functional Theory to Engineers and Scientists — **Kristen Fichthorn, Michael J. Janik, Lasse Jensen, Jorge Sofo, Adri van Duin**

**4:10 Paper 710d:** Software Strategies for Increasing Throughput and Reproducibility While Lowering Cognitive Load in Molecular Simulation — **Eric Jankowski, Stephen Thomas, Michael Henry**

**4:25 Paper 710e:** Reproducible Computational Workflows with Signac — **Carl Simon Adorf, Paul M. Dodd, Vyas Ramasubramani, Bradley Dice, Sharon C. Glotzer**

**4:40 Paper 710f:** Making Data-Driven *in silico* Research a Mainstream Chemical Engineering Tool — **Johannes Hachmann**

**4:55 Paper 710g:** Open Chemistry, Avogadro and Jupyter: User Friendly Frontends — **Marcus D. Hanwell**

**5:10 Paper 710h:** COMSOF Workbench: Tools for Efficient Coarse-Grained Modeling of Soft Materials — **Frederick R. Phelan Jr., Brian Moroz**

**5:25 Paper 710i:** MoSDeF: Molecular Simulation and Design Framework for Transparent, Reproducible, Usable By Others, Extensible Simulations (TRUE) — **Peter T. Cummings, Justin Gilmer, Christoph Klein, János Sallai, Andrew Z. Summers, Chris Iacovella, Ákos Lédeczi, Peter Volgyesi, Clare McCabe**

#### **(711) Modeling and Engineering Cellular Communities**

**Thursday, Nov 1, 3:30 PM**  
Westin Convention Center, Westmoreland East

Rajib Saha, Chair  
Pushkar Lele, Co-Chair

**Sponsored by:** Bioengineering

**3:30 Paper 711a:** Predicting the Spatially Differential Gut Microbiota Composition Using Genome-Scale Metabolic Modeling — **Siu Hung Joshua Chan, Margaret Senftle, Costas D. Maranas**

**3:48 Paper 711b:** Elucidating Microbiome-Virome Interactions and Metabolic Transactions in Bovine Rumen through *in silico* genome-Scale Modeling — **Mohammad Mazharul Islam, Samodha C. Fernando, Rajib Saha**

**4:06 Paper 711c:** Understanding the Stability and Robustness of a Methanotroph-Cyanobacterium Coculture through Kinetic Modeling and Experimental Verification — **Kiumars Badr, Matthew Hilliard, Q. Peter He, Jin Wang**

**4:24 Paper 711d:** Tools for Engineering Coordinated System Behaviour in Synthetic Microbial Consortia — **Nicolas Kyllis, Zoltan A. Tuza, Guy-Bart Stan, Karen Polizzi**

**4:42 Paper 711e:** Rapid Isolation, Phenotyping, and Engineering of Microorganisms from the Rat Gut Targeting d-Amino Acid Production — **Tong Si, Huimin Zhao, Jonathan V. Sweedler**

**5:00 Paper 711f:** Engineered Substrate Specificity for Prebiotic Control of Microbial Community Population and Gene Expression — **Fatima Enam, Emily Kramer, Thomas J. Mansell**

**5:18 Paper 711g:** Metabolic Mechanisms of Interaction in Cellular Communities — **Jason Papin**

#### **(712) Nanobiotechnology for Sensors and Imaging II**

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 311  
Daniel Roxbury, Chair

**Sponsored by:** Bionanotechnology

**3:30 Paper 712a:** Invited Speaker: Real Time, Label Free Biosensing *in-Vivo* Using Single Walled Carbon Nanotubes and Other Carbon Nanomaterials — **Michael Strano**

**3:50 Paper 712b:** Graphene Based Sensing Platform for Studying Amyotrophic Lateral Sclerosis — **Bijentimala Keisham, Akop Seksenyan, Steven Denyer, Pouyan Kheirkhah, Gregory Arnone, Pablo Avalos, Abhiraj D. Bhimani, Clive Svendsen, Vikas Berry, Ankit Mehta**

**4:06 Paper 712c:** Xeno Nucleic Acids for Enhancing the Optical Stability of Nanosensors — **Alice Gillen, Justyna Kupis-Rozmyslowicz, Carlo Gigli, Nils Schuergers, Ardemis A. Boghossian**

**4:22 Paper 712d:** Quantification of Inflammatory Response and Morphological Change of SIM-A9 Microglia By Neuro-Probes — **Darwin Yang, Markita Landry**

**4:38 Paper 712e:** Aggregation State Determines Uptake, Intracellular Processing, and Long-Term Fate of Single-Walled Carbon Nanotubes in Mammalian Cells — **Mitchell Gravely, Daniel Roxbury**

**4:54 Paper 712f:** Semi-Rational Design of Steroid Biosensors Using Compositionally Controlled Corona Phase Molecular Recognition: Pathway Towards *In Vivo* Monitoring — **Michael A. Lee, Song Wang, Naveed Bakh, Crystal Pham, Kelvin K. Jones, Freddy T. Nguyen, Gili Bisker, Michael Strano**

**5:10 Paper 712g:** Substrate Functionalized Carbon Nanotubes As a Modular Tool for Tracking Soil Enzyme Activity — **Nathaniel Kallmyer, Erica Peterson, Nigel Reuel**

**5:26 Paper 712h:** Evolution of Nanoparticle-Based Synthetic Molecular Recognition — **Sanghwa Jeong, Anneliese Gest, Markita Landry**

**5:42 Paper 712i:** Development of Hydrogel Encapsulated Carbon Nanotube Based Biomonitoring System and Its Applications Toward the Detection of Riboflavin Administration — **Naveed Bakh, Michael A. Lee, Freddy T. Nguyen, Xun Gong, Gili Bisker, Michael Strano**

**(713) New Technologies to Enhance the Production of Unconventional Oil and Natural Gas: Simulation****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 321

Jared Ciferno, Chair  
Rameshwar Srivastava, Co-Chair  
Jason Tremblay, Co-Chair**Sponsored by:** Advances in Fossil Energy R&D**3:30 Paper 713a:** Numerical Simulation of Natural Fractures on EOR By Cyclic Gas Injection in Unconventional Reservoirs Using Dfn — **Chongwei Xiao, Olatoyosi Obilade****3:55 Paper 713b:** Enhancing Hydraulic Fracturing Productivity Via Model-Based Feedback Control — **Prashanth Siddhamshetty, Joseph Sangil Kwon****4:20 Paper 713c:** Numerical Analysis of Hydrocarbon Flow in Shale Gas Reservoirs — **Mohammad Hatami, Alireza Sarvestani, David J. Bayless****4:45 Paper 713d:** Approximate Semi-Analytical Solution for a Penny-Shaped Rough-Walled Hydraulic Fracture Driven By Turbulent Fluid in an Impermeable Rock — **Navid Zolfaghari****5:10 Paper 713e:** A Reduced Order Model for Optimizing Hydraulic Fracture Stimulation of Horizontal Wells — **Cheng Cheng, Andrew P. Bunger****5:35 Paper 713f:** Prototype LIBS Sensor for Sub-Surface Water Quality Monitoring — **Jinesh Jain, Dustin McIntyre, Daniel Hartzler****(714) Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications II****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 413

Georgios A. Sotiriou, Chair  
Timothy Brenza, Co-Chair**Sponsored by:** Nanoparticles**3:30 Paper 714a:** Enzyme-Mimetic Luminescent Luminescent Nanoparticles As Hydrogen Peroxide Biosensors — **Georgios A. Sotiriou****4:10 Paper 714c:** Targeted Single-Walled Carbon Nanotubes for Photothermal Ablation of Breast Cancer Combined with Immunostimulation — **Patrick McKernan, Rajagopal Ramesh, Linda Thompson, Roger Harrison****4:30 Paper 714d:** Effect of Ethanol Solvent on Antimicrobial Efficiency of Magnesium Oxide Nanoparticles — **Proma Bhattacharya, Sudarsan Neogi****4:50 Paper 714e:** Synthesis and Optical Characterization of Gadolinium-Containing Scintillating Nanoparticles to Enable Neural Stimulation — **Ashley Dickey, Eric Zhang, Stephen H. Fougler, Joseph W. Kolis****5:10 Paper 714f:** Synthesis, Characterization and Antibacterial Study of Copper-Nickel Bimetallic and Mixed Metal Oxide Nanocomposite — **Debashri Paul, Sudarsan Neogi****(715) Planning and Scheduling II****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 409

Zukui Li, Chair  
Iiro Harjunoski, Co-Chair**Sponsored by:** Computers in Operations and Information Processing**3:30 Paper 715a:** Adaptive Scheduling of Steelmaking and Continuous Cast Process Under Uncertainty — **Sanjula Kammammettu, Zukui Li****3:49 Paper 715b:** A Rolling Horizon Scheduling Algorithm Considering Electricity Load Tracking and Future Load Prediction — **Giancarlo Dalle Ave, Iiro Harjunoski, Sebastian Engell****4:08 Paper 715c:** Comparison of Risk-Averse Stochastic Programming and Adaptive Robust Optimization: A Virtual Power Plant Scheduling Application — **Ricardo M. Lima, Antonio Conejo, Loïc Giraldo, Olivier Le Maître, Ibrahim Hoteit, Omar Knio****4:27 Paper 715d:** Novel Formulation for Optimal Schedule with Demand Side Management in Multi-Product Air Separation Processes — **Shengnan Zhao, M. Paz Ochoa, Ignacio E. Grossmann, Lixin Tang, Irene Lotero, Ajit Gopalakrishnan****4:46 Paper 715e:** Multi-Operational Development Planning for Multi-System Shale Gas Production — **Abigail Ondeck, Markus G. Drouven, Nathan Blandino, Ignacio E. Grossmann****5:05 Paper 715f:** Continuous-Time Scheduling Formulation for Pipeline Systems with Branches — **Pedro M. Castro, Hossein Mostafaei****5:24 Paper 715g:** Preprocessing Algorithms and Tightening Constraints for Blend Scheduling Models — **Yifu Chen, Christos T. Maravelias****5:43 Paper 715h:** Long-Term Maintenance and Production Planning for the Integrated Chemical Enterprise — **Satyajith Amaran, Sreekanth Rajagopalan, Mark Joswiak, Scott J. Bury****(716) Polyelectrolytes and Polymer Electrolytes****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 327

Vivek Sharma, Chair  
Allie Obermeyer, Co-Chair**Sponsored by:** Polymers**3:30 Paper 716a:** PEG-Based Polyampholytes As Cryopreservatives — **Nathaniel A. Lynd, Aaron A. Burkey, Taylor Hatridge****3:45 Paper 716b:** Ion Specific Effects in Charged Polymers for Membrane Applications — **Yuan Yuan Ji, Hongxi Luo, Geoffrey M. Geise****4:00 Paper 716c:** Extensional Relaxation Time, Pinch-Off Dynamics and Printability of Semi-Dilute Polyelectrolyte Solutions — **Leidy N. Jimenez, Jelena Dinic, Vivek Sharma****4:15 Paper 716d:** Salt Permeation Mechanisms through Inkjet Printed Charge Mosaic Membranes — **Mark J. Summe, Sushree Jagriti Sahoo, William A. Phillip****4:30 Paper 716e:** Coarse-Grained Simulations of Weak Polyacid Titration in Explicit Salt — **Vikramjit S. Rathee, Jonathan K. Whitmer****4:45 Paper 716f:** The Effect of Charge Monomer Sequence in Complex Coacervation — **Tyler Lytle, Charles E. Sing****5:00 Paper 716g:** Structure and Rheology of Polyelectrolyte Complex Coacervates — **Amanda B. Marciel, Samanvaya Srivastava, Matthew V. Tirrell****5:15 Paper 716h:** Sequence and Structure Effects in the Complex Coacervation of Proteins with Polyions — **Rachel Kapelner, Nicholas Zervoudis, Allie Obermeyer****5:30 Paper 716i:** Partitioning and Enhanced Self-Assembly of Actin in Polypeptide Coacervates — **Samanvaya Srivastava, Patrick McCall, Sarah L. Perry, David Kovar, Margaret L. Gardel, Matthew V. Tirrell****5:45 Paper 716j:** Characterization of Thermoresponsive Polyelectrolyte Complex Micelles — **Sachit Shah, Lorraine Leon****(717) Polymer Characterization****Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 326

Keith M. Forward, Chair  
Blair Kathryn Brettmann, Co-Chair**Sponsored by:** Polymers**3:30 Paper 717a:** A Composition-Morphology Mapping of Particle-Filled Polymer Blends up to High Fill Fraction — **Derrick Amoabeng, David Roell, Kendal Clouse, Brian A. Young, Sachin Velankar****3:45 Paper 717b:** Mathematical Aspects of Modeling the Rheology of Complex Material — **Matthew Armstrong, Geoffrey Bull, Jeffrey S. Horner, Antony N. Beris****4:00 Paper 717c:** The Complex Role of Entanglements and Associations in Supramolecular Self-Healing — **Zachary R. Hinton, Aamir Shabbir, Nicolas J. Alvarez****4:15 Paper 717d:** Volume Fraction Dependence of Linear Viscoelasticity of Starch Suspensions — **Jinsha Li, Prasuna Desam, Vivek Narsimhan, Osvaldo Campanella, Ganesan Narsimhan****4:30 Paper 717e:** Rheology of Novel Blends Containing Polybutylene / Linear Low Density Polyethylene Composites — **Bader H. Al-Busairi, Mariam Awad****4:45 Break****5:00 Paper 717g:** Thermal Transport and Flow in Polymeric Materials — **David Venerus, David Nieto Simavilla, Andy Kiessling, Jay D. Schieber****5:15 Paper 717h:** A Novel Self-Dispersed  $\beta$  Nucleating Agent for Isotactic Polypropylene and Its Unique Nucleation Behavior and Mechanism — **Shicheng Zhao****5:30 Paper 717i:** Pressure-Sensitive Adhesives Based on Strain-Activated Crosslinking of Functional Groups — **Yen Tran, John Klier, Shelly Peyton****5:45 Paper 717j:** Surface Functionalization of Porous Substrates Via Initiated Chemical Vapor Deposition — **Christine Cheng, Malancha Gupta**

**(718) Polymer Networks and Gels**  
**Thursday, Nov 1, 3:30 PM**  
 David L. Lawrence Convention Center, 330

Nese Orbey, Chair  
 Samanvaya Srivastava, Co-Chair

**Sponsored by:** Polymers

**3:30 Paper 718a:** Studying the Toughening Mechanism of Mussel-Inspired Iron-Catechol Complexes in Epoxy Networks — **Thomas R. Cristiani**, Emmanouela Filippidi, Claus D. Eisenbach, J. Herbert Waite, Jacob Israelachvili, B. Kollbe Ahn, Megan T. Valentine

**3:45 Paper 718b:** Detecting Bond Breakage and Fracture in Tough Hydrogels — **Gabriel E. Sanoja**, Rint P. Sijbesma, Costantino Creton

**4:00 Paper 718c:** Dynamic Networks As Multi-Stimuli Responsive Actuating Adhesives — **Deborah K. Schneiderman**, Forrest S. Etheridge, Qiong Wu, Amy S. Metlay, Brian T. Michal, Stuart J. Rowan

**4:15 Paper 718d:** Biomolecules for Non-Biological Things: Materials Construction through Peptide Design and Solution Assembly — **Darrin J. Pochan**

**4:45 Paper 718e:** Dynamically Responsive Microcapsules from Microfluidic Complex Emulsion Drop Templating — **Jörg G. Werner**, Saraf Nawar, Zhang Wu, David A. Weitz

**5:00 Paper 718f:** Non-Isocyanate Low Temperature Curing Sprayed Applied Automotive Decorative Topcoat — **Yaqi Wo**, Paul Lamers, Hyun Wook Ro, Xiangling Xu, Diane Wargo, Gina Bonnett, David Fenn, Caroline Harris, Shanti Swarup, Matthew Luchansky

**5:15 Paper 718g:** Super-Stretchable Polymeric Elastomers with Healable Mechanical Property and Recoverable Gas-Separation Functionality — **Pengfei Cao**, Bingrui Li, Tao Hong, Zhe Qiang, Konstantinos Vogiatzis, Alexei Sokolov, Tomonori Saito

**5:30 Paper 718h:** Mesoscopic Structure of Semi-Crystalline Vitrimers: The Remarkable Case of Polyethylene — **Ralm Ricarte**, François Tournilhac, Ludwik Leibler

**5:45 Paper 718i:** “Smart” Applications of Stimuli-Responsive Hydrogels — **Siowling Soh**

**(719) Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals**  
**Thursday, Nov 1, 3:30 PM**  
 Westin Convention Center, Fayette

Christopher H. Marton, Chair  
 Moiz Diwan, Co-Chair

**Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum

**3:30 Paper 719b:** Exploring the Kinetics of API Degradation Under Hot Melt Extrusion Conditions — **Anuj A. Verma**, Kushal Sinha, Moiz Diwan

**3:55 Paper 719c:** Towards Predicting the Quality of HME Products — **Josip Matic**, Carolina Alva, Hannes Bauer, Johannes G. Khinast

**4:20 Paper 719d:** A Predictive Transport Model for Drying of Polymer Strip Films — **Alireza Naseri**, Eylül Cetindag, Joseph Forte, **Ecevit Bilgili**, Rajesh Davé

**4:45 Paper 719e:** High Shear Wet Granulation Scale-up Study Using Discrete Element Modeling — **Maitraye Sen**, Jonathan Brett Wade, Salvador García-Muñoz, James E. Miesle, Mark Schrad

**5:10 Paper 719f:** Predicting Shear, Energy Dissipation, and Blending in Bioreactors for Mammalian Cells — **Brian DeVincendis**, John A. Thomas, Kevin Smith

**5:35 Paper 719g:** Simulation of Industrial-Scale Aerated Bioreactors — **Christian Witz**, Philipp Eibl, Johannes G. Khinast

**(720) Quantitative Approaches to Disease Mechanisms and Therapies**  
**Thursday, Nov 1, 3:30 PM**  
 Westin Convention Center, Butler

Stacey D. Finley, Chair  
 David Rumschitzki, Co-Chair  
 Carolyn Harris, Co-Chair

**Sponsored by:** Engineering Fundamentals in Life Science

**3:30 Paper 720a:** Integrative Mathematical Model to Investigate Chemotherapy Induced Peripheral Neuropathy through a Mechanistic Study of Neuronal Dynamics — **Parul Verma**, Doraiswami Ramkrishna

**3:48 Paper 720b:** Mechanistic Assessment of the Effect of Phthalates and Heavy Metals on Neurodevelopment — **Dimosthenis Sarigiannis**, Nafsika Papaioannou, Maria Fafouti, Michael Dickinson, Kinga Polanska, Aikaterini Gabriel, Spyros Karakitsios

**4:06 Paper 720c:** Intracellular Absorption Underlies Collective Bacterial Tolerance Towards an Antimicrobial Peptide — **Fan Wu**, Cheemeng Tan

**4:24 Paper 720d:** Targeting Phospholipid Metabolism to Prevent Hepatocyte Lipotoxicity — **Sarah A. Sacco**, Alexandra K. Leamy, Jamey D. Young

**4:42 Paper 720e:** *In Vitro* and *In Silico* Characterization of Human Nasal Epithelial Pathophysiology in Cystic Fibrosis Airway Disease — **Florencio Serrano Castillo**, Timothy Corcoran, Carol A. Bertrand, William J. Confer, Monica E. Shapiro, Robert S. Parker

**5:00 Paper 720f:** Calmodulin Stabilizes Camkii Autophosphorylation through Structural Exclusion of Phosphatase — **Matthew Pharris**, Tyler VanDyk, Scott Bolton, Melanie Stefan, Tamara L. Kinzer-Ursem

**5:18 Paper 720g:** Invited Speaker: Modeling How Brain Cells Form Networks in Health and Disease — **Amina A. Qutub**

**(721) Reactions in Near-Critical and Supercritical Fluids**  
**Thursday, Nov 1, 3:30 PM**

David L. Lawrence Convention Center, 404

Hema Ramsurn, Chair  
 Michael T. Timko, Co-Chair  
 Wang-Ting (Grace) Chen, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**3:30 Paper 721a:** Characterization of Flow and Heat Transfer Parameters in a Continuous Flow Hydrothermal Liquefaction Reactor — **Feng Cheng**, Travis Le-Doux, Brian Trefitz, Scott Woolf, Sergio Guillen, Jacob Usrey, Cesar A. Martinez Bejarano, Hengameh Bayat, Umakanta Jena, Catherine E. Brewer

**3:47 Paper 721b:** Hydrothermal Liquefaction of Model Polysaccharides and Polysaccharide-Rich Food-Processing Waste — **Akhila Gollakota**, Azin Padash, John Kaplan, Phillip E. Savage

**4:04 Paper 721c:** Capturing the Phase Interface Using the Gradient Theory in the Mixing of Hydrocarbons and Supercritical Water — **Ping He**, Arash Azimi, Ashwin Raghavan, Ahmed F. Ghoniem

**4:21 Paper 721d:** Study of the Catalytic Reactions of Ethylene Oligomerization in Subcritical and Supercritical Media over a Nibea Catalyst — **Gabriel Seufitelli**, Fernando Resende

**4:38 Paper 721e:** Effect of Heterogeneous Catalysts on Upgrading Quality of Bio-Crude Under Sub- and Super-Critical Water Conditions — **Kodanda Phani Raj Dandamudi**, Connor Copp, Tessa Murdock, Peter Lammers, Shuguang Deng

**4:55 Paper 721f:** Challenges of Designing a Short Residence Time Hydrothermal Continuous Reactor for Algae Processing — **Ashani Samararatunga**, Mason Martin, Orlando Ayala, Sandeep Kumar

**5:12 Paper 721g:** Hydrothermal Degradation of Hormones and Antibiotics — **Nepu Saha**, M. Toufiq Reza

**5:29 Paper 721h:** Influence of Solvents on Metal Contents in Biocrude Oil from Hydrothermal Liquefaction of Microalgae — **Jimeng Jiang**, Phillip E. Savage

**(722) Soft Matter Electrokinetics**  
**Thursday, Nov 1, 3:30 PM**  
 Omni William Penn Hotel, Conference Center A

Christopher L. Wirth, Chair  
 Ning Wu, Co-Chair

**Sponsored by:** Interfacial Phenomena

**3:30 Paper 722a:** Electric Double Layers: Effect of Asymmetry in Electrolyte Valence on Finite Ion Size Effects, Dielectric Decrement and Ion-Ion Correlations — **Ankur Gupta**, Pawel J. Zuk, Howard A. Stone

**3:46 Paper 722b:** The Breakup of an Oil Drop Containing a Colloidal Suspension in an Electric Field — **Rajarshi Sengupta**, Javier Lanaute, Lynn M. Walker, Aditya S. Khair

**4:02 Paper 722c:** Electroacoustic Colloidal Assembly in a Continuous Flow-through Microfluidic Device — **Jaime Juárez**, Meghana Akella

**4:18 Paper 722d:** Electric-Field Driven Assembly of Polarizable Colloids Confined to a Surface — **Joseph Maestas**, Ning Wu, David T. Wu

**4:34 Paper 722e:** An Immersed Boundary Method for Rapid Dynamic Simulation of Electrokinetic Phenomena in Dispersions of Nanoparticles in Concentrated Electrolytes — **Zachary Sherman**, James Swan

**4:50 Paper 722f:** Shaped-Directed Dynamics of Active Colloids Powered By Induced-Charge Electrophoresis — **Allan M. Brooks**, Syeda Sabrina, Kyle J. M. Bishop



**5:06 Paper 722g:** Drop in "Additives" for Suspension Manipulation — **Anirudha Banerjee, Todd M. Squires**

**5:22 Paper 722h:** Shape-Directed Dynamics of Active Colloids Powered By Contact Charge Electrophoresis — **Yong Dou, Kyle J. M. Bishop**

**5:38 Paper 722i:** Controlled Synthesis of Organic Nano/Micro-Wires on Gold Nanoparticle Seeds for Sensors Applications — **Xuecheng Yu, Mohamed Kilani, Evan Schaefer, Guangzhao Mao**

**(723) Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond II**

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 302

Fang Wang, Chair  
Marina Tsianou, Co-Chair  
Xiaobin Jiang, Co-Chair

**Sponsored by:** Crystallization and Evaporation

**3:30** Introductory Remarks

**3:35 Paper 723a:** Spatial Confined Capillary Flow and Precisely Controlled Crystallization Via 3D Printed Platform: A Comprehensive View — **Mingguang Han, Gaohong He, Xiaobin Jiang**

**3:55 Paper 723b:** Polymorph Screening of L-Glutamic Acid By Anti-Solvent Crystallization in Easy-to-Use Microfluidic Device — **Huanhuan Shi, Xin Huang, Hongxun Hao**

**4:15** Break

**4:55 Paper 723e:** Thermodynamics of Co-Crystal Systems — **Dipali Ahuja, Ake Rasmuson**

**5:15 Paper 723f:** Investigations on Co-Milling of Pharmaceutical Cocrystals Via Characterization and Physico-Chemical Stability Evaluation — **Rahamatullah Shaikh, Eoin Sheehan, Jacek Zeglinski, Denise Croker, Gavin Walker**

**(724) Sustainable Energy: Generation and Storage**

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 317

Sheila Samsatli, Chair  
Vilas G. Pol, Co-Chair

**Sponsored by:** Sustainable Energy

**3:30 Paper 724a:** Low-CO<sub>2</sub> Integrated Networks for Heat and Electricity Based on Hydrogen: A Comprehensive Spatio-Temporal MILP Model for Planning, Design and Operation of Future Value Chains — **Sheila Samsatli**

**3:48 Paper 724b:** Membrane-Free Water Splitting for Hydrogen Generation — **Avigail Landman**

**4:06 Paper 724c:** Replicating Indian Point's Energy Generation Using Renewable Energy Pathways: A Technical and Economic Stochastic Analysis — **Jenny Frank, Tristan Brown, Robert Malmshiemer, Marie-Odile Fortier, Timothy A. Volk, Rohit Bhonagiri, Kirsten McGiver**

**4:24** Break

**4:42 Paper 724e:** Ultra-High Thermal Effusivity Materials for Resonant, Ambient Thermal Energy Harvesting — **Anton L. Cottrell, Albert Tianxiang Liu, Volodymyr Koman, Michael Strano**

**5:00 Paper 724f:** Comparative Evaluation of Lead Emissions and Toxicity Potential in the Cradle-to-Gate Life Cycle of Lead Halide Perovskite Photovoltaics — **Pieter Billen, Enrica Leccisi, Subham Dastidar, Siming Li, Liliana Lobaton, Sabrina Spataro, Aaron T. Fafarman, Vasilis M. Fthenakis, Jason B. Baxter**

**5:18 Paper 724g:** Preparation of Lithium Ion Battery Cathode Composites Using Leonardite-Derived Humic Acid — **Xiaodong Hou, Yong Hou, Michael Mann, Justin Baker**

**5:36 Paper 724h:** A Novel Dynamic Simulation Methodology for High Temperature Packed-Bed Thermal Energy Storage — **Jacob F. Tuttle, Nate White, Kody Powell**

**(725) Synthetic Biology Applications**

**Thursday, Nov 1, 3:30 PM**  
Westin Convention Center, Westmoreland West-Central

Nikhil U. Nair, Chair  
Kang Wu, Co-Chair  
J. Andrew Jones, Co-Chair

**Sponsored by:** Bioengineering

**3:30 Paper 725a:** A Hysteretic Mammalian Genetic Circuit for Detection of Proteasomal Degradation — **Yimeng Zeng, Tram Nguyen, Laura Segatori**

**3:48 Paper 725b:** Discovering a Tomato Natural Product Biosynthetic Pathway Using an Integrated Synthetic Biology Approach — **Sijin Li, Christina D. Smolke**

**4:06 Paper 725c:** Engineering Red Blood Cell-Based Biosensors for Physiological Monitoring — **Taylor Dolberg, Kelly A. Schwarz, Joshua N. Leonard**

**4:24 Paper 725d:** Engineering Synergistic Interactions between Antibiotics and Sequence-Specific Gene Expression Treatment to Re-Sensitize Multi-Drug Resistant Bacteria — **Peter Otoupal, Keesha Erickson, Kristen Eller, Thomas Aunins, Anushree Chatterjee**

**4:42 Paper 725e:** A Semi-Synthetic Regulatory Infrastructure Can Remodel Yeast Global Phenotypic State for Rapid Growth on Non-Native Nutrients of Choice — **Vikas Trivedi, Venkatesh Endalurgopinarayanan, Nikhil U. Nair**

**5:00 Paper 725f:** A Robust Light-Driven CO<sub>2</sub> to Limonene Conversion By a Synthetic Microbial Consortium — **Shrameeta Shinde, Kaya Mernitz, Xin Wang**

**5:18 Paper 725g:** Taking Any Molecule from Any Microbe from the Lab to Full-Scale Manufacturing — **Ute Galm**

**(726) Value-Added Co-Products from Biorefineries**

**Thursday, Nov 1, 3:30 PM**  
David L. Lawrence Convention Center, 316

Blake A. Simmons, Chair  
Rebecca Ong, Co-Chair  
Justinus Satrio, Co-Chair

**Sponsored by:** Sustainable Biorefineries

**3:30 Paper 726a:** Effects of Co-Product Uses on Environmental and Economic Sustainability of Hydrocarbon Biofuel from One- and Two-Step Pyrolysis of Poplar — **Daniel Kulas, Olumide Winjobi, Wen Zhou, David R. Shonnard**

**3:55 Paper 726b:** Optimizing Alkaline-Oxidative Pretreatment of Hybrid Poplar to Maximize Lignin Co-Product Value — **Sandip Kumar Singh, Thanaphong Phongpreecha, ZhaoYang Yuan, Eric Hegg, David Hodge**

**4:20 Paper 726c:** Controlled Radical Polymerization of Lignin-Derived Bio-Oil for Melt-Spinable Thermoplastic — **Wangda Qu, Yuerui Huang, Eric W. Cochran, Xianglan Bai**

**4:45 Paper 726d:** Lignin Nanoparticles (LNPs) Fabrication through Tailored Lignin Reactivity By Innovative Sequential Organosolv Fragmentation Approach (ISOFA) — **Zhi-Hua Liu, Arthur J. Ragauskas, Joshua Yuan**

**5:10 Paper 726e:** Production of 2,5-Furan Dicarboxylic Acid (FDCA) in Ionic Liquid Media — **Ravikumar Gogar, Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi**

**5:35 Paper 726f:** Converting Switchgrass into Cellulosic Sugars, Lipids, and Carotenoids — **Zhu Chen, Caixia Wan**

## (727) Water Treatment, Desalination, and Reuse II

Thursday, Nov 1, 3:30 PM

David L. Lawrence Convention Center, 304

Ngoc Bui, Co-Chair

Jamie Hestekin, Co-Chair

Oishi Sanyal, Co-Chair

**Sponsored by:** Membrane-Based Separations

**3:30 Paper 727a:** Membrane Mineral Scaling in Semi-Batch and Steady State Reverse Osmosis Desalination - a Comparative Study — **Tae Lee, Anditya Rahardianto, Yoram Cohen**

**3:52 Paper 727b:** Water Desalination and Purification through Mixed-Matrix Membranes: An Atomistic Simulation Study — **Zeyu Zhao, Jianwen Jiang**

**4:14 Paper 376bc:** Metal Oxide Functionalized Graphene Oxide Membranes for Advanced Oxidation of Pollutants — **Ashish Aher, Mainak Majumder, Dibakar Bhattacharyya**

**4:36 Paper 727d:** Enhanced Biocidal and Antifouling Properties of Thin Film Composite Membranes Via Active Layer Modification with Polyrhodanine Nanoparticles — **Ahmad Arabi Shamsabadi, Ahmad Rahimpour, S. Fatemeh Sayedpour, Masoud Soroush**

**4:58 Paper 727e:** Modifying TiO<sub>2</sub> Magnéli Phase Reactive Electrochemical Membranes with Pyrogenic Carbonaceous Materials for Adsorption and Electrochemical Removal of Water Contaminants — **Soroush Almassi, Brian Chaplin**

**5:20 Paper 727f:** Quantification of Thermal Energy Delivery to Water-Membrane Interface in Membrane Distillation — **Alexander Dudchenko, Mukta Hardikar, Ruikun Xin, Alaina Anand, Shounak Joshi, Meagan Mauter**

**5:42 Paper 727g:** Ceramic Membranes for Desalination By a Vacuum Flow-through Evaporation — **Shailesh Dangwal, Ruochen Liu, Rita Anam Epse M, Christopher Groesbeck, Seok-Jhin Kim**

## (728) Advances in Data Analysis and Information Management

Friday, Nov 2, 8:00 AM

David L. Lawrence Convention Center, 311

Franjo Cecelja, Chair

Xiaonan Wang, Co-Chair

**Sponsored by:** Data and Information Systems

**8:00 Paper 728a:** Ensemble Models for Univariate Time Series Forecasting — **Brad Johnson, Nick Sahinidis**

**8:19 Paper 728b:** Ontology Engineering Approach to Support Process of Model and Data Integration — **Linsey Koo, Edlira Kalemi, Franjo Cecelja**

**8:38 Paper 728d:** Conceptual Modelling for Integrated Decision-Making in Process Systems — **Canan Dombayci, Antonio Espuña**

**8:57 Paper 728e:** Comparison of Surrogate Modeling Techniques for Surrogate-Based Optimization — **Bianca Williams, Selen Cremaschi**

**9:16 Paper 728f:** Semantic Networking Facility for the Biorefining Community — **Edlira Kalemi, Linsey Koo, Franjo Cecelja**

**9:35 Paper 728g:** The Use of Asset-Oriented Data Models for Data Integration Enables Advanced Analytics in the Process Industry — **Mark C. Molaro**

**9:54 Paper 728h:** Parameter Prediction for Stochastic Job Shop Scheduling Using Probabilistic Machine Learning — **Teemu Ikonen, Iiro Harjunkoski**

## (729) Bio-Based Polymers

Friday, Nov 2, 8:00 AM

David L. Lawrence Convention Center, 319

Shudipto Konika Dishari, Chair

Joseph F. Stanzione III, Co-Chair

**Sponsored by:** Polymers

**8:00 Paper 729a:** Wood Nanotechnologies — **Liangbing Hu**

**8:30 Paper 729b:** Fabrication of Biodegradable Corn Zein Films with Varying Hydrophobic/Hydrophilic Balance Using Different Contact Surfaces and Treatment with SF<sub>6</sub> Plasma — **Morgan Malm, Jozef Kokini**

**8:45 Paper 729c:** Fabrication and Decoration of Zein-Based Electrospun Nanofiber Platforms for SERS Detection — **Hazal Turasan, Miko Cakmak, Jozef Kokini**

**9:00 Paper 729d:** Grazing Incidence X-Ray Scattering Reveals Texturing in Plant Cell Walls — **Sintu Rongpipi, Dan Ye, Sarah Kiemle, Chenhui Zhu, Daniel Cosgrove, Esther W. Gomez, Enrique D. Gomez**

**9:15 Paper 729e:** Improving Mechanical Properties of Fatty Acid-Derived Thermoplastic Elastomers By Incorporating a Transient Network — **Wenyue Ding, Megan Robertson**

**9:30 Paper 729f:** Physical State of Dry Native Cellulose in Solution with Ionic Liquids — **Nyalaliska Utomo, Behzad Nazari, Sujyot Mony, Indira Saifuddin, Ralph H. Colby**

**9:45 Paper 729g:** Preparation of Microalgal EPS/PVA Blend Nanofibers for Waste Water Remediation — **Adarsh Bafana, Shishir V Kumar, Prasad P Pawar, Ashiqur Rahman, Si Amar Dahoumane, Clayton S Jeffryes**

**10:00 Paper 729h:** Dipeptide-Based Polyphosphazene Polymers for Regenerative Engineering — **Kenneth S. Ogueri, Jorge Luis Escobar Ivirico Sr., Lakshmi S. Nair, Harry R. Allcock, Cato T. Laurencin**

**10:15 Paper 729i:** Bio-Based Thermosets Prepared Using Michael Addition of Furan and Isosorbide Building Blocks — **Xi Chu, John La Scala, Giuseppe Palmese**

## (730) Catalytic Processing of Fossil and Biorenewable Feedstocks III: Furan Chemistry

Friday, Nov 2, 8:00 AM

David L. Lawrence Convention Center, 315

Basudeb Saha, Chair

James W. Harris, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 730a:** Catalytic Hydrogenation of Furfural over Rumop: Probing Bimetallic and Compositional Effects on Catalyst Performance — **Yolanda Bonita, Timothy O'Connell, Jason C. Hicks**

**8:18 Break**

**8:36 Paper 730c:** Etherification of 5-Hydroxymethylfurfural Using Zeolite Catalysts — **Meredith Allen, Spencer Martell, Akbar Mahdavi Shakib, William M. Gramlich, Brian G. Frederick, Thomas J. Schwartz**

**8:54 Paper 730d:** Mechanistic Insights into the Hydrogenolysis of Levoglucosan over Bifunctional Platinum Silica-Alumina Catalysts in Tetrahydrofuran Solvent — **Siddarth H. Krishna, Rajeev Assary, Quinn A. Rashke, Zachary R. Schmidt, Larry Curtiss, James A. Dumesic, George W. Huber**

**9:12 Paper 730e:** Hydrothermal Stability of Chloromethyl Polystyrene Based Solid Acid Catalysts and Mechanism of Cellulose Hydrolysis — **Maksim Tyufekchiev, Jordan Finzel, Pu Duan, Klaus Schmidt-Rohr, Sergio Granados-Focil, Marion Emmert, Michael T. Timko**

**9:30 Paper 730f:** Glycerol Transfer-Hydrogenation of Levulinic Acid Using Ru and Ir Carbene Organometallics Immobilized on Active Hydrotalcites — **Jacob Heltzel, Kai Wang, Matthew Finn, Evan Sandefur, Adelina Voutchkova-Kostal**

**9:48 Paper 730g:** Paired Electrocatalytic Hydrogenation and Oxidation of 5-Hydroxymethylfurfural for Efficient Production of Biorenewable Monomers — **Xiaotong Chadderdon, David Chadderdon, Wenzhen Li**

**10:06 Paper 730h:** A Full Furfural Utilization over Ni/SiO<sub>2</sub> Catalysts — **Sheng-Chiang Yang, Shawn D. Lin**

### (731) Crosslinked Polymers

Friday, Nov 2, 8:00 AM

David L. Lawrence Convention Center, 320

Samanvaya Srivastava, Chair  
Nese Orbey, Co-Chair

**Sponsored by:** Polymers

**8:00 Paper 731a:** Surface-Attached Orthogonal Gradient Networks — **Pandiyarajan Chinnayan Kannan**, Michael Rubinstein, Jan Genzer

**8:15 Paper 731b:** An Versatile Reactive UV Stabilizer for Biodegradable Poly(butylene adipate-co-terephthalate) Films — **Qianqiu Xing**

**8:30 Paper 731c:** Development of Novel Crosslinked Polymers for the Capture and Sensing of Environmental Pollutants — **Rishabh Shah**, Thomas Dziubla, James Z. Hilt

**8:45 Paper 731d:** Hexaarylbiimidazole-Derived Lophyl Radicals As Latent, Long-Lived Reactive Species in Cross-Linked Polymers — **Timothy F. Scott**, Austin Bingham, Dowon Ahn, Scott Zavada

**9:00 Paper 731e:** Effect of Cross-Linking on CO<sub>2</sub>-Induced Plasticization Resistance of Polyimides Containing DABA Diamine - a Molecular Simulation Study — **Marcel Balçık**, Sadiye Velioglu, S. Birgül Tantekin-Ersolmaz, M. Goktug Ahunbay

**9:15 Paper 731f:** BIG Dipper Dynamic Contact Angle Curves for Pt-Cure PDMS Gradients — **Kayesh Ashraf**, Chenyu Wang, Sithara Nair, Kenneth J. Wynne

**9:30 Paper 731g:** Development and Characterization of Soluble Polyphenolic Poly(beta amino ester) Polymers for Single Step Nanoparticle Formulations — **Kelley Wiegman**, J. Zach Hilt, Thomas Dziubla

**9:45 Paper 731h:** Reprocessable Polyhydroxyurethane Network Composites: Effect of Filler Surface Functionality on Reprocessability and Stress Relaxation Behavior — **Xi Chen**, Lingqiao Li, John M. Torkelson

**10:00 Paper 731i:** Monodisperse Elastomeric Microparticle Scaffolds for Heterogeneous Palladium-Mediated Catalysis — **Jeffrey A. Bennett**, Jan Genzer, Milad Abolhasani

**10:15 Paper 731j:** Novel Amphoteric Cryogels for Sr<sup>2+</sup> and Cs<sup>2+</sup> Ions Removal from Aqueous Solutions — **Vassilis J. Inglezakis**, Stavros Pouloupoulos, Alzhan Baimenov, Dmitry Berillo

### (732) Fundamentals of Catalysis IV: Surface Reactivity

Friday, Nov 2, 8:00 AM

David L. Lawrence Convention Center, 318

Tej S. Choksi, Chair  
Derek Falcone, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**8:00 Paper 732a:** Accurate Adsorbate Free Energies from First-Principles — **Prateek Mehta**, Anshumaan Bajpai, Kurt Frey, Andrew Lehmer, Gray Laughlin, William F. Schneider

**8:18 Paper 732b:** Defining and Counting Site Requirements for Reactions on Curved and Crowded Surfaces — **David Hibbitts**, Abdulrahman S. Almithn, David W. Flaherty, Jianwei Liu, Enrique Iglesias

**8:36 Paper 732c:** Tuning the Surface Reactivity of Intermetallic Compounds Towards Carbon, Oxygen, and Hydrogen to Affect CO vs. CO<sub>2</sub> Production in Wet Reforming of Hydrocarbons and Oxygenates — **Yuanjun Song**, Yang He, Siris Laursen

**8:54 Paper 732d:** Amination of 1-Hexanol over Au-Pd/TiO<sub>2</sub> Catalysts Prepared By Controlled Surface Reactions — **Madelyn R Ball**, Thejas S. Wesley, Keishla R. Rivera-Dones, George W. Huber, James A. Dumesic

**9:12 Paper 732e:** Structure Sensitivity Analysis of Propane Dehydrogenation(PDH) on Palladium Alloys — **Ranga Rohit Seemakurthi**, Fabio H. Ribeiro, Jeffrey Greeley

**9:30 Paper 732f:** Adsorption and Reaction of Furfuryl Alcohol on Pt(111): A Comparison Study to Pd(111) — **Lesli Mark**, Alexander H. Jenkins, Hendrik Heinz, Will Medlin

**9:48 Paper 732g:** Kinetics and Mechanism of Aspartic Acid Adsorption and Its Explosive Decomposition on Cu(100) — **Burcu Karagoz**, Aaron Reinicker, A.J. Gellman

**10:06 Paper 732h:** Density Functional Theory Study of the Effect of Step Edges on  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Surfaces on Cl-Surface Interactions and the Cl-Induced Depassivation Process — **Qin Pang**, Hossein DorMohammadi, O. Burkan Isgor, Liney Arnadottir

### (733) Modeling and Computation in Energy and Environment

Friday, Nov 2, 8:00 AM

David L. Lawrence Convention Center, 310

Yash Puranik, Chair  
Liwen Chen, Co-Chair  
Ping He, Co-Chair  
Joseph Sangil Kwon, Co-Chair

**Sponsored by:** Applied Mathematics and Numerical Analysis

**8:00 Paper 182c:** Two Stage Stochastic Programming Modeling Approach for Energy Storage System Operation Under Uncertainty — **Jiah Yu**, Jun-Hyung Ryu, In-Beum Lee

**8:19 Paper 733b:** Theoretical and Experimental Investigation of the Microbial Degradation of Solitary Oil Microdroplets — **George E. Kapellos**, Nicolas Kalogerakis, Patrick S. Doyle

**8:38 Paper 733c:** Modeling Faradaic Capacitive Deionization with Redox Active Porous Electrodes — **Fan He**, P. M. Biesheuvel, Martin Z. Bazant, T. Alan Hatton

**8:57 Paper 733d:** Resilient and Sustainable Bioenergy Systems Modelling — **Miao Guo**

**9:16 Paper 733e:** Finding the Ideal Feedstock for Biodiesel Production Via Generalized Kinetic Model for Transesterification and Saponification — **Pulkit Chhabra**, Markus Kraft, Iftekhar A. Karimi, Anikesh Kumar

**9:35 Paper 733f:** Accelerating the Generation of Coal Power Plant Property Models — **Benjamin Sauk**, Nick Sahinidis

**9:54 Paper 733g:** Dynamic Optimisation of Water-Injection Wells Operation for Enhanced Oil Production from a Mature Oil and Gas Field — **Emmanuel Epelle**, Dimitrios I. Gerogiorgis

**10:13 Paper 733h:** Voluntary Oil Well Ignition As a Blowout Response: Analysis of Factors Influencing Viability — **A. Rashid Hasan**, Joseph Sangil Kwon, Prashanth Siddhamshetty, M. Sam Mannan, Boyue Xu, Monir Ahammad

### (734) Modeling, Control, and Optimization of Energy Systems

Friday, Nov 2, 8:00 AM

David L. Lawrence Convention Center, 309

Alexander W. Dowling, Chair  
John D. Hedengren, Co-Chair

**Sponsored by:** Systems and Process Control

**8:00 Paper 734a:** Multi-Objective and Dynamic Real-Time Optimization of Postcombustion Carbon Capture Processes for Cycling Applications — **Rebecca Kim**, Fernando V. Lima

**8:17 Paper 734b:** Dynamic Modeling and Control of a Post-Combustion Solid-Sorbent Capture System with the Ccsi Models and Tools — **Benjamin P. Omell**, Priyadarshi Mahapatra, Debangsu Bhattacharyya, David C. Miller

**8:34 Paper 734c:** Application of a Data-Driven Modeling Approach to a Large-Scale Power Plant — **Seyed Mostafa Safdarnejad**, Jacob F. Tuttle, Kody Powell

**8:51 Paper 734d:** Model-Based Analysis of a Thermofluidic Engine for Low-Grade Heat Recovery: Accounting for Irreversible Thermal Losses — **Yukun Wang**, Christos N. Markides, Benoit Chachuat

**9:08 Paper 734e:** Model Predictive Control Designs to Achieve Uniform Growth of Simultaneously Propagating Multiple Fractures in Hydraulic Fracturing — **Prashanth Siddhamshetty**, Kan Wu, Joseph Sangil Kwon

**9:25 Paper 734f:** Real-Time Control and Balancing of a Reformer Furnace — **Anh Tran**, Marquis Crose, Madeleine Pont, Panagiotis D. Christofides

**9:42 Paper 734g:** Finite Element Modeling and Optimization of Heat Exchangers — **Saif R. Kazi**, Lorenz T. Biegler

**9:59 Paper 734h:** Application of Paroc in the Optimization and Control of PEM Water Electrolysis Process — **Stratos Pistikopoulos**, Gerald S. Ogumerem

**10:16 Paper 734i:** Predictive Control of Solar Collector Energy System with Gaussian Process Priors of Uncertain Solar Irradiance — **Xiaodong Xu**, Yuan Yuan, Stevan Dubljevic



**(735) Modeling of Biomaterials****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 321

Yi He, Co-Chair  
Qing Shao, Co-Chair  
Reid Van Lehn, Co-Chair**Sponsored by:** Biomaterials**8:00 Paper 735a:** Computational Studies on Modeling, Simulating and Designing Amyloid Biomaterials — **Sai Vamshi R Jonnalagadda**, Chrysoula Kokotidou, Graziano Deidda, Eirini Ornthopoulou, Asuka A. Orr, Hae-Kwon Jeong, Anna Mitraki, Phanourios Tamamis**8:18 Paper 735b:** Self-Assembly of Amyloid Peptide Fragments with Experiment Directed Simulations — **Dilnoza Amirkulova**, Maghesree Chakraborty, Andrew White**8:36 Paper 735c:** Investigating the Role of Phosphorylation and pH in Peptide Binding to Silica — **Kayla Sprenger**, Arushi Prakash, Gary Drobny, Jim Pfandtnr**8:54 Paper 735d:** Surface Interaction between Short-Chain Cellulosic Polymers and Cellulose Nanocrystals from Molecular Simulation — **Naveen Kumar Vasudevan**, Li Xi**9:12 Paper 735e:** A Simple Model for Understanding Friction between Biomaterial Surfaces — **Nan Xu**, Shen Tan, Tao Xia, **Yi He****9:30 Paper 735f:** Self-Assembly of Amphiphilic Nanosheets Based on Grafted Polymeric Triangular-Plate in Selective Solvents — **Xianyu Song**, Shuangliang Zhao, Jiabo Tao, Xia Han, Honglai Liu**9:48 Paper 735g:** Coarse-Grained Simulations to Understand the Mechanisms Underlying Ring Formation in Methylcellulose — **Vaidyanathan Sethuraman**, Kevin D. Dorfman**10:06 Paper 735h:** Diffusion and Concentration Profiles for Loading DL-Propanolol in a Crosslinked Drug Carrier, Poly(N-isopropyl acrylamide) Hydrogel — **Hajar Taheri Afarani**, Holly A. Stretz, John Massingill Jr., Tania Betancourt**(736) Multiphase Reaction Engineering****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 316

Xinrui Yu, Chair  
Vaibhav Kelkar, Co-Chair  
Onkar Manjrekar, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**8:00 Paper 736a:** Experimental and Modeling Study of Passive NO<sub>x</sub> Adsorption: Pd-Exchanged-ZSM-5 — **Mugdha Ambast**, Kyle Karinshak, Michael Harold**8:22 Paper 736b:** Kinetics of the Solid-Liquid Transesterification to Produce Sucrose Esters Using Sodium Stearate As Contacting Agent — **Maria F. Gutierrez**, Alvaro Orjuela, Tapio Salmi, Dmitry Yu. Murzin**8:44 Paper 736c:** Model-Based Equipment Design for the Biphasic Production of 5-Hydroxymethylfurfural in a Tubular Reactor — **Maximilian Aigner**, Andreas Jupke**9:06 Paper 736d:** Exploring the Contribution of Liquid in the Pore Network of Sorbent Polymer Composite Materials on Hg Removal from Flue Gas — **Vladimiro Nikolakis**, Uwe Beuscher, Michael McCutchen, Vineet Rakesh**9:28 Paper 736e:** Modeling of Biodiesel Production in Liquid-Liquid Film Reactors Including Mass Transfer Effects — **Mario Andres Noriega**, Paulo C. Narvaez, Alberto Claudio Habert**9:50 Paper 736f:** Understanding Super Acidic Molten Salt Hydrate Media for Cellulose Hydrolysis — **Natalia Rodriguez Quiroz**, Dionisios G. Vlachos**10:12 Paper 736g:** Probing the Reacting Interface of a Liquid-Liquid Cu-Free Sonogashira Coupling — **Benjamin Rizkin**, **Ryan L. Hartman****(737) Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 302

Joshua Engstrom, Chair  
Lofli Derdour, Co-Chair**Sponsored by:** Crystallization and Evaporation**8:00 Paper 737a:** 02B07 Introductory Remarks — **Joshua Engstrom****8:05 Paper 737b:** Thermodynamic Properties of Paracetamol Impurities and Their Impact on the Crystallisation of Paracetamol from Solution — **René R. E. Steendam**, Leila Keshavarz, Brian de Souza, Patrick Frawley**8:25 Paper 737c:** A Novel Approach into Secondary Nucleation and Crystal Growth, Controlled Particle Size Distribution, Using a Large Single Seed Crystal in Solution Crystallization — **Mustafa Yousuf**, P.J. Frawley**8:45 Paper 737d:** Crystal Growth Kinetics of Salicylamide Investigated Under Different Crystallisation Processes and Also Environmental Conditions — **Aisling Lynch**, Ake Rasmuson**9:05 Paper 737f:** Fast Temperature Cycling via Microwave Heating Enables Enhanced Deracemization — **Christos Xiouras**, Fabio Cameli, G. D. Stefanidis**9:25 Paper 737g:** Resolution of Conglomerates Using Preferential Crystallization and Enzymatic Racemization — **Thiane Carneiro**, Shashank Bhandari, Katarzyna Wrzosek, Erik Temmel, Heike Lorenz, Andreas Seidel-Morgenstern**9:45 Paper 737h:** Alkaline Crystallization of CaCO<sub>3</sub> in a Direct Air Capture Process — **Caroline E. Giacomini**, Luisa Burhenne, Walter Mérida**(738) Pyrolysis of Biomass****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 317

Fernando Resende, Chair  
Hsi-Wu Wong, Co-Chair  
Hsu Chiang, Co-Chair**Sponsored by:** Catalysis and Reaction Engineering Division**8:00 Paper 738a:** Bench-scale Measurement of Pyrolysis Products from Intact Live Fuels — **Mohammad-Saeed Safdari**, Jansen Berryhill, David R. Weise, Thomas Fletcher**8:22 Paper 738b:** The Kinetic and Chemistry of Biomass Fast Pyrolysis Using Novel Micro-Sphere Micro-Reactor Technology — **Ali Zolghadr**, Joseph J. Biernacki**8:44 Paper 738c:** Networks with Parallel and Sequential Reactions for Determining the Pyrolysis Kinetics of Biomass Feedstocks — **Ye Gao**, Kyriacos Zygorakis**9:06 Paper 738d:** Design, Construction and Conceptual Proof of a Free Fall Fast Pyrolysis Reactor — **Diana C. Vargas**, Jhoselyn Padilla, Cristina Arciniega, Kevin M. Van Geem, Daniela Almeida Streitwieser**9:28 Paper 738e:** Reaction Paths for Hemicellulose Pyrolysis Using Reactive Molecular Dynamics — **Amrutha Raghuram**, Phillip R. Westmoreland**9:50 Paper 738f:** Enthalpy Changes during Pyrolysis of Biomass: Interpretation of Intraparticle Gas Sampling — **Marco J. Castaldi**, Simona Ciuta, Francesco Patuzzi, Marco Baratieri**10:12 Paper 738g:** Ex-Situ Catalytic Fast Pyrolysis of Beetle Killed Lodgepole Pine in Novel Ablative Reactor — **Heather Wise**, Fernando Resende, Anthony Dichiera

**(739) Recent Advances in Molecular Simulation Methods II****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 305

Erik E. Santiso, Chair  
Andrew White, Co-Chair  
Harish Vashisth, Co-Chair**Sponsored by:** Computational Molecular Science and Engineering Forum**8:00 Paper 739a:** Dissipative Particle Dynamics Simulations of Anion Exchange Membranes — **Ming-Tsung Lee****8:15 Paper 739b:** Computational Investigation of Water Desalination across Nanofiltration Membranes Using Advanced Sampling Techniques — **Hessam Malmir, Razi Epsztein, Menachem Elimelech, Amir Haji-Akbari****8:30 Paper 739c:** Combining Biased Sampling and Markov State Models to Characterise the Assembly and Exchange Dynamics of Molecular Materials in Solution — **Veselina Marinova, Loukas Kollias, Ilaria Gimondi, Matteo Salvalaglio****8:45 Paper 739d:** In silico Prediction of Structural Properties of Racemic Porous Organic Cage Crystals — **Yang Liu, David S. Sholl****9:00 Paper 739e:** NMR Relaxation from Molecular Simulations: Study on Bulk Hydrocarbons and Water — **Arjun Valiya Parambathu, Dilip Asthagiri, Philip Singer, George J. Hirasaki, Walter G. Chapman****9:15 Paper 739f:** Densities and Viscosities of H<sub>2</sub>S at Elevated Pressures and Temperatures Using Molecular Dynamics Simulations — **Abhinav Verma, Rajdeep S. Payal, Indranil Rudra, S Balasubramanian****9:30 Paper 739g:** Greenhouse Gas Capture: A Recent Theoretical Advancement — **Anwesa Karmakar, Enrique R. Batista, Ping Yang****9:45 Paper 739h:** Exploring the Effect of Mutations on Thermodynamic and Enzymatic Properties of Cyclophilin 40 — **Mert Gur, Elizabeth A. Blackburn, Jia Ning, Vikram Narayan, Kathryn L. Ball, Malcolm D. Walkinshaw, Burak Erman****10:00 Paper 739i:** Mechanisms of Synthetic Chloride Ion Transporters in Lipid Bilayer Membranes — **J. Patrick Brian, Vance Jaeger****10:15 Paper 739j:** Understanding the Molecular Physiology of the Blood-Brain Barrier Tight Junctions — **Shikha Nangia****(740) Solid-Fluid Separations in Oil & Gas Production and Refining Processes****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 303

Seyi Oduyungbo, Chair  
Isaac Gamwo, Co-Chair**Sponsored by:** Fluid-Particle Separations**8:00 Paper 740a:** Centrifugal Filtration of Solvent Diluted Bitumen from Oil Sands — **Merouane Khammar, Yuming Xu****8:25 Paper 740b:** Integrated Forward Osmosis-Membrane Distillation Process for Sustainable Treatment of High Tds Produced Waters — **S. Ranil Wickramasinghe, Peter Fyfe, Kamyar Sardari****8:50 Paper 740c:** Optimizing Sand Control in Wellhead with Advanced De-Sander Technology — **Banchao Shu, Oluwatosin Oyelakin, Priyanka Shahi, Isaac Snyder, Mike Fredrick, Jeevan Dahal****(741) Thermophysical Properties of Biological Systems****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 307

Phanourios Tamamis, Chair  
Jens Glaser, Co-Chair**Sponsored by:** Thermodynamics and Transport Properties**8:00 Paper 741a:** Multiscale Modeling of Stratum Corneum Lipid Mixtures — **Christopher R. Iacovella, Timothy C. Moore, Parashara Shamprasad, Annette L. Bunge, Clare McCabe****8:25 Break****8:50 Paper 741c:** Molecular Dynamics of Volatile Organic Compounds in the Epicuticle of Plant Epidermal Cells — **Shaunak Ray, Natalia Dudareva, John A. Morgan****9:15 Paper 741d:** Modeling the Self-Assembly of Super-Charged Green Fluorescent Proteins — **Jens Glaser, Vyas Ramasubramani, Anna J Simon, David W. Taylor, Andrew D. Ellington, Sharon C. Glotzer****9:40 Paper 741e:** Proteins at Extreme Conditions: From Understanding Life to Practical Applications — **Betul Uralcan, Pablo G. Debenedetti****10:05 Paper 741f:** High-Resolution Structural Studies of Protein Directed Nanomaterial Synthesis — **Brent L. Nannenga, Amar Thaker****(742) Thermophysical Properties: Theory and Experiments for Charged Systems****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 306

Erik E. Santiso, Chair  
Clare McCabe, Co-Chair  
Sanket A. Deshmukh, Co-Chair**Sponsored by:** Thermodynamics and Transport Properties**8:00 Paper 742a:** Liquid-Liquid Phase Separation of Ionic Liquids By Water Addition (Experiment and Simulation) — **M. Alejandra Rocha, Yong Zhang, Edward J. Maginn, Mark B. Shiflett****8:19 Paper 742b:** The Effect of Selective Fluorination on the Structure and Thermodynamics of Ionic Liquids — **Jeremy Hurst, Joshua Strickland, Brooks D. Rabideau****8:38 Paper 742c:** Molecular Simulation Investigation of Pure and Mixed Gas Absorption in a Non-Ideal Binary Ionic Liquid Mixture — **Utkarsh Kapoor, Atiya Banerjee, Jindal K. Shah****8:57 Paper 742d:** Properties of Ionic Liquids and Other Solvents Containing Functionalities Based on Glycerol Skeletons — **Shuai Qian, Kathryn E. O'Harra, Grayson P. Dennis, Tristin A. Jones, Jason E. Bara****9:16 Paper 742e:** Computational Studies of Absorption Refrigeration Systems Using Mixtures of Refrigerants, Ionic Liquids and Deep Eutectic Solvents — **Rubaiyet Abedin, Sharareh Heidarian, John C. Flake, Francisco R. Hung****9:35 Paper 742f:** Phase Behavior of the Primitive Model of Ionic Liquid in the Slit Pore: A Density Functional Approach with the Association Concept — **Kun Liu, Jianzhong Wu****9:54 Paper 742g:** Revisiting Theories and Conventions of Electrolyte Thermodynamic Models — **Xi Yang, George M. Bollas****10:13 Paper 742h:** Understanding and Improving the (Al,Sc)N Heterostructural Alloy through DFT Calculations and Combinatorial Synthesis — **Samantha L. Millican, Kevin Talley, Alan W. Weimer, Andriy Zakutayev, Charles B. Musgrave, Geoff Brennecke, Aaron M. Holder****(743) Water Treatment, Desalination, and Reuse III****Friday, Nov 2, 8:00 AM**

David L. Lawrence Convention Center, 304

Jeffrey McCutcheon, Co-Chair  
Christine Duval, Co-Chair  
Seetha Manickam, Co-Chair**Sponsored by:** Membrane-Based Separations**8:00 Paper 743a:** Exploration of Polysaccharide Derivatives-Based Anionic Polyelectrolytes As Novel Draw Solutes in Forward Osmosis — **Chun Ding, Yan Wang****8:21 Paper 743b:** Assessing the Selective Adsorption of Contaminants Using Spectroscopy and Chemometrics — **Reginald E. Rogers Jr., Cody Cummings, Hayley K. Richardson, Paula M. Zaretsky, Todd Pagano****8:42 Paper 743c:** Functionalized Poly(methacrylic acid) Membranes with Bimetallic Nanoparticles: From Bench Scale to Water Remediation Applications — **Hongyi Wan, Sebastián Hernández, Nicolas Briot, M. S. Islam, Lindell Ormsbee, Dibakar Bhattacharyya****9:03 Paper 743d:** Effect of Membrane Surface Chemistry on Grafting Density and Molecular Weight Cutoff — **Nima Shahkaramipour, Chong Cheng, Haiqing Lin****9:24 Paper 743e:** Cost Optimization of Osmotically Assisted Reverse Osmosis — **Timothy Bartholomew, Nicholas Siefert, Meagan Mauter****9:45 Paper 743f:** Investigating Graphene Oxide and Holey Graphene Oxide Membrane Properties for Water Purification — **Ali Alshami, Chris Buelke****10:06 Paper 743g:** Advanced Electrokinetic Desalination for Brackish Water: Water and Energy Nexus — **Shu-Yuan Pan, Seth W. Snyder, Aaron I. Packman, Yupo J. Lin, Pen-Chi Chiang**

**(744) Catalytic Upgrading of Alternative Carbon Feedstocks**

**Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 315

David Hibbitts, Chair

Thomas J. Schwartz, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 744a:** Aqueous Phase Reforming of Glycerol: Determining the Catalyst Support Effects

— **Torrie Sewell**, Rachel B. Getman, David A. Bruce

**12:48 Paper 744b:** Catalytic Amino Acid Production from Biomass

— **Ning Yan**

**1:06 Paper 744c:** Renewable Lubricant Alkanes from Biomass-Derived Platform Chemicals — **Angela M. Norton**, Sibao Liu, Basudeb Saha, Dionisios G. Vlachos

**1:24 Paper 744d:** Identification of Active Sites for Selective C-O Cleavage Reactions on Metals Supported on Reducible Oxides — **Lawrence Barrett**, Nicholas M. Briggs, Alejandra Gomez, Valeria Herrera, Taiwo Oмотoso, Steven Crossley

**1:42 Paper 744e:** CO<sub>2</sub> Hydrogenation on Single-Site Heterogeneous Cobalt Catalyst — **Juan Jimenez**, Cun Wen, Jochen Lauterbach

**2:00 Paper 744f:** Coupled CO<sub>2</sub> Capture and Conversion to Methanol Using Solid Sorbents with a Homogeneous Catalyst — **Elizabeth A. K. Wilson**, Shawn C. Eady, Trent Silbaugh, Mark Barteau, Levi T. Thompson

**2:18 Paper 744g:** Selective CO<sub>2</sub> Hydrogenation to Methanol over Promoted Indium-Based Catalysts — **Chen-Yu Chou**, Raul F. Lobo

**2:36 Paper 744h:** Enhancement of Catalytic Performance of Ordered Mesoporous “One-Pot” Fe-Al<sub>2</sub>O<sub>3</sub> Catalysts By Ni Incorporation in Dry Reforming of Biogas — **Karam Jabbour**, Ali Saad, Lena Inati, Anne Davidson, Pascale Massiani, Nissrine El Hassan

**(745) Fundamentals of Catalysis V**

**Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 316

Dante Simonetti, Chair

Eleni A. Kyriakidou, Co-Chair

**Sponsored by:** Catalysis and Reaction Engineering Division

**12:30 Paper 745a:** Kinetic Evaluation of N<sub>2</sub> Activation in Plasma Catalytic Ammonia Synthesis — **Patrick Barboun**, Prateek Mehta, Francisco Herrera, David Go, William F. Schneider, Jason C. Hicks

**12:48 Paper 745b:** Atomically Dispersed Supported Metal Catalysts: Tuning Catalytic Performance with Supports and Ionic Liquid Coatings — **Melike Babucci**, Chia-Yu Fang, Adam Hoffman, Alexey Boubnov, Simon R. Bare, Bruce C. Gates, Alper Uzun

**1:06 Paper 745c:** Effects of Water on the Kinetics of Acetone Hydrogenation over Metal Catalysts — **Benginur Demir**, Ashwin Chemburkar, Thomas Kropp, Manos Mavrikakis, Matthew Neurock, James A. Dumesic

**1:24 Paper 745d:** Ab-Initio Study of the Interface between g-Al<sub>2</sub>O<sub>3</sub> and Pt — **Kofi Oware Sarfo**, Arielle L. Clauser, Liney Amadottir, Melissa K. Santala

**1:42 Paper 745e:** Molten Salt Hydrates As Solvents in the Synthesis of Metal Oxide Catalysts — **Trang Tran**, Yuanhao Yu, Justin Marlowe, George Tsilomelekis

**2:00 Paper 745f:** Kinetics Investigation of Ethanol Dehydration and Dehydrogenation over a Model Oxide Catalyst — **Hussein T. Abdulrazzaq**, Thomas J. Schwartz

**2:18 Paper 745g:** DFT Studies of Intermetallic Gamma-Brass Structured Catalysts for Selective Hydrogenation — **Haoran He**, Anish Dasgupta, Randall J. Meyer, Robert Rioux, Michael Janik

**2:36 Paper 745h:** Stability of Pt Nanoparticles Supported on γ-Al<sub>2</sub>O<sub>3</sub> during *in Situ* Reduction/Oxidation — **Henry Ayoola**, Matthew McCann, Matthew Curman, Wissam A. Saidi, Judith C. Yang

**(746) Gas Hydrates Science and Engineering**

**Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 307

Amadeu K. Sum, Chair

Praveen Linga, Co-Chair

**Sponsored by:** Thermodynamics and Transport Properties

**12:30 Paper 746a:** The State of the Art Prototype Design for Clathrate Hydrate Based Desalination (HyDesal) Process Utilizing LNG Cold Energy — **Ponnivalavan Babu**, Abhishek Nambiar, Praveen Linga

**12:45 Paper 746b:** Detection and Characterization of Gas Hydrate Deposition in Deadlegs Under Water Saturated Gas — **Jeong-Hoon Sa**, Bo Ram Lee, Xianwei Zhang, Keijo Kinnari, Kjell Askvik, Xiaoyun Li, Torstein Austvik, Kjetil Folgerø, Kjetil Haukalid, Jan Kocbach, Amadeu Sum

**1:00 Paper 746c:** Evaluation of CO<sub>2</sub>/C<sub>3</sub>H<sub>8</sub> Gas Mixture for Clathrate Hydrate Based Desalination (HyDesal) Process — **Ponnivalavan Babu**, Abhishek Nambiar, Praveen Linga

**1:15 Paper 746d:** Development of Ozone Hydrate Generation System — **Tomomi Hatsugai**, Ryutaro Nakayama, Ryo Akiyoshi, Shirou Nishitsuka, Ryo Nakamura, Yasuaki Ryoukuta, Ryo Ohmura

**1:30 Paper 746e:** Stability Assessment of Hydrate Pellets for Energy Storage — **Hari Prakash Veluswamy**, Asheesh Kumar, Praveen Linga

**1:45 Paper 746f:** Characterization of Hydrate-Water Anti-Adhesion Under Surface-Active Agents — **Wonhyeong Lee**, Juwon Min, Seungjun Baek, Yun-Ho Ahn, Jae W. Lee

**2:00 Paper 746g:** Developing Nanoparticles As Anti-Agglomerant for Gas Hydrate Slurry Flow — **Xianwei Zhang**, Jingjing Gong, Ning Wu, Amadeu Sum

**2:15 Paper 746h:** Numerical Simulation of Hydrates in Porous Media for Clathrate Based Applications — **Maninder Khurana**, Praveen Linga

**2:30 Paper 746i:** Diffusion of Methane in SI Hydrates: A Kinetic Monte Carlo and Theoretical Study — **Lee Shin Chu**, David T. Wu, Shiang-Tai Lin

**2:45 Paper 746j:** A Model for Gas-Hydrate Equilibrium in Porous Media — **Patricia Taboada-Serrano**, Yali Zhang

**(747) Integrated Product and Process Design**

**Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 311

Mariano Martin, Chair

Ravendra Singh, Co-Chair

**Sponsored by:** Systems and Process Design

**12:30 Paper 747a:** Fragrance Product Design/Screening Methods Using an Integrated Machine Learning and Camd Model — **Lei Zhang**, Haitao Mao, Linlin Liu, Jian Du, Rafiqul Gani

**12:49 Paper 747b:** Optimal Production of Power from Mid-Temperature Geothermal Sources: Scale and Safety Issues — **Javier Peña-Lamas**, Juan Martínez-Gómez, Mariano Martin, José M. Ponce-Ortega

**1:08 Paper 747c:** Computer-Aided Reaction Solvent Design Integrated with New Reaction Mechanism Model — **Qilei Liu**, Lei Zhang, Linlin Liu, Jian Du, Qingwei Meng

**1:27 Paper 747d:** Reactor Network Development for Rigid Polyols Production — **Yunhan Wen**, Lorenz T. Biegler, Jeff Ferrio

**1:46 Paper 747e:** Mixed Integer Linear Programming Optimization Framework Applied to a Platinum Group Metals Flotation Circuit — **Eric Tswaledi Mabotha**, Cornelius Mduduzi Masuku

**2:05 Paper 747f:** Simultaneous Working Medium Selection, Process and Control System Design for Organic Rankine Cycles — **Theodoros Zarogiannis**, Alexios S. Kyriakides, Athanasios I. Papadopoulos, Panos Seferlis

**2:24 Paper 747g:** Process Optimization-Centric Design and Screening of Nanoporous Adsorbents for Gas Separations — **Shachit S. Iyer**, Ishan Bajaj, M. M. Faruque Hasan

**2:43 Paper 747h:** Universal Graph Structures for Property Estimation — **Charles C. Solvason**, Russell Burnett



**(748) Modeling, Estimation, and Identification****Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 309

Daniel Chen, Chair  
Kirti Yenkie, Co-Chair**Sponsored by:** Systems and Process Control**12:30 Paper 748a:** Estimating Parameters and Model Uncertainty in Fundamental Dynamic Models Using Historical Data — **Kimberley B. McAuley**, Hadiseh Karimi**12:49 Paper 748b:** Accommodating Missing, Non-Uniformly Sampled and Delayed Measurements for Modeling and Control of Variable Duration Batch Processes in a Subspace Identification Framework — **Abhinav Garg**, Prashant Mhaskar**1:08 Paper 748c:** Investigation of CO<sub>2</sub> Sorption Mechanisms in Isothermal Columns Via Transient Material and Energy Flow PDE Models — **Manda Yang**, Linxi Wang, Seyed Mehdi Kamali Shahri, Robert M. Rioux, **Antonios Armaou****1:27 Paper 748d:** Output Feedback Regulation Via Carleman Based Receding Horizon Estimation and Control — **Yizhou Fang**, **Antonios Armaou****1:46 Paper 748e:** Adaptive Control of System with Unknown Inputs with Application to Chemical Reaction Control — **B. Erik Ydstie**, Zixi Zhao**2:05 Paper 748f:** Optimization of Heterogeneous Batch Reactor Under Parameter Uncertainty — **Yajun Wang**, Mukund Patel, John M. Wassick, Lorenz T. Biegler**2:24 Paper 748g:** Estimating the Drainage Area of "Frac-HIT" or Refractured Horizontal Well — **Nitish Goyal**, Matteo Marongiu-Porcu, **Michael Nikolaou****2:43 Paper 748h:** Thin Falling Film Layer Monitoring and State Estimation Via Discrete Kuramoto-Sivashinsky Observer and Kalman Filter — **Junyao Xie**, **Stevan Djuljevic****(749) Real-Time Optimization of Operations****Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 310

Dimitrios Varvarezos, Chair  
Ali Mesbah, Co-Chair**Sponsored by:** Computers in Operations and Information Processing**12:30 Paper 749a:** A Generalized State-Space Model for Online Scheduling — **Dhruv Gupta**, **Christos T. Maravelias****12:49 Paper 749b:** Integration of Automation Logic and Scheduling for Real-Time Batch Chemical Plant Optimization — **Venkatachalam Avadiappan**, Blake C. Rawlings, **Christos T. Maravelias**, **Stephane Lafortune**, John M. Wassick, **William Edsall**, Adam Kelloway, Bao Lin, **Naresh N. Nandola**, **Mathias Hakenberg****1:08 Paper 749c:** Dynamic Real-Time Optimization of a Coal-Fired Power Plant Using an Artificial Neural Network Model — **Jacob F. Tuttle**, **Mostafa Safdarnejad**, Kody Powell**1:27 Paper 749d:** Efficient Real Time Optimization Using Approximate Dynamic Programming — **Jasper Kelly**, **Isaac Oboka**, **Yu Yang****1:46 Paper 749e:** An Overview and Evaluation of Approaches for Online Process Optimization — **Dinesh Krishnamoorthy**, **Bjarne Foss**, **Sigurd Skogestad****2:05 Paper 749g:** Accelerated Parallel Alternating Method of Multipliers (ADMM) for Distributed Optimization — **Wentao Tang**, **Prodromos Daoutidis****2:24 Paper 749h:** Dynamic Modeling for Improved Operation and Control of a Supercritical CO<sub>2</sub> Brayton Power Cycle — **Stephen E. Zitney**, **Eric A. Liese**, **Priyadarshi Mahapatra**, **Jacob Albright****(750) Recent Advances in Force Fields****Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 306

Andrew White, Chair  
Erik E. Santiso, Co-Chair  
Harish Vashisth, Co-Chair**Sponsored by:** Thermodynamics and Transport Properties**12:30 Paper 750a:** Simple Molecular Reactive Force Field - a Novel Approach to Capturing Bond-Making and-Breaking — **Henry C. Herbol**, **Paulette Clancy****12:45 Paper 750b:** Rational Development of Reactive Force Fields — **Roland Faller****1:00 Paper 750c:** Achieving Large Scale Quantum-Accurate Reactive Molecular Dynamics: The Chebyshev Interaction Model for Efficient Simulations (ChIMES) — **Rebecca Lindsey**, **Laurence E. Fried**, **Sorin Bastea**, **Nir Goldman****1:15 Paper 750d:** Sticking Efficiency of Polyaromatic Hydrocarbons at High Temperatures By Reactive Molecular Dynamics — **Eirini Goudeli**, **Christopher J. Hogan Jr.****1:30 Paper 750e:** Building Better Water Force Fields: A Systematic and Reproducible Optimization of 3- and 4-Point Water Models with an Improved Nonbonded Functional Form — **Joseph S. Gomes**, **Vijay Pande****1:45 Paper 750f:** An Accurate Force Field for Graphitic Materials Including Virtual Pi Electrons and Applications to Understand Carbon Nanotube Dispersion in Solvents and Polymer Solutions — **Chandrani Pramanik**, **Jacob Gissinger**, **Satish Kumar**, **Hendrik Heinz****2:00 Paper 750g:** A Hybrid Approach Toward Systematically-Derived Implicit-Solvent Coarse-Grained Lipid Models — **Alexander J. Pak**, **Thomas Dannenhoffer-Lafage**, **Jesper J. Madsen**, **Gregory A. Voth****2:15 Paper 750j:** Improved Directional Hydrogen Bonding Interactions for the COSMO-SAC Model for Prediction of Activity Coefficients — **Chun-Kai Chang**, **Wei-Lin Chen**, **David T. Wu**, **Shiang-Tai Lin****(751) Techniques for Removing Fine and Ultrafine Particles from Gaseous, Aqueous or Non-Aqueous Media****Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 303

Seyi Oduyungbo, Chair  
Hseen O. Baled, Co-Chair**Sponsored by:** Fluid-Particle Separations**12:30 Paper 751a:** Filtration of Multi-Component Aerosols Using Polymeric Nanofiber Membranes — **Junli Hao**, **Saptarshi Chattopadhyay**, **Gregory C. Rutledge****12:55 Paper 751b:** Dynamic Split Flow Separation of Micron-Sized Slurry Fischer-Tropsch Catalyst Particles — **Udaya Bhaskar Reddy Ragula****1:20 Break****1:45 Paper 751d:** High Throughput in Situ Cultivation and Isolation of Unculturable Bacteria Using Microfluidic Devices — **Clara Romero Santiveri**, **Francesca Ispaso**, **Edgar D. Goluch****(752) Water Treatment, Desalination, and Reuse IV****Friday, Nov 2, 12:30 PM**

David L. Lawrence Convention Center, 304

Isabel Escobar, Co-Chair  
William A. Phillip, Co-Chair  
Mahdi Malmali, Co-Chair**Sponsored by:** Membrane-Based Separations**12:30 Paper 752a:** Interfacial Transport in Nanocellulose-Based Nanocomposite Membranes for Improved Reverse Osmosis Performance — **Ethan D. Smith**, **Keith Hendren**, **Jacob Haag**, **Earl J. Foster**, **Stephen M. Martin****12:50 Paper 752b:** Predictive Models for Ion Removal in Brackish Water Desalination Using Electrodialysis Process — **Leila Karimi**, **Abbas Ghassemi****1:10 Paper 752c:** Separation of Oil-in-Water Emulsions Stabilized By Different Types of Surfactants Using Electrospun Fiber Membranes with Surface Modification — **Yi-Min Lin**, **Gregory C. Rutledge**

**1:30 Paper 752d:** Methods for Direct Surface Temperature Measurement for Quantification of Membrane Distillation Process Performance — *Alexander Dudchenko, Meagan Mauter*

**1:50 Paper 752e:** A Simple Approach for Functionalization of Poly(vinylidene fluoride) (PVdF) Membranes for Desalination of Oil-Contaminated Saline Water Using Membrane Distillation — *Mahdi Mohammadi Ghalei, Abdullah Al Balushi, Mona Bavarian, Siamak Nejati*

**2:10 Paper 752f:** In-Situ pH Control for Selective Removal of Toxic Elements to Sustain Water Supply for Cooling and Process Water — *Yupo J. Lin, Lauren Valentino, Manvitha Marni, Aaron I. Packman*

**(753) Unconscious Bias**  
**Monday, Oct 29, 8:00 AM**  
David L. Lawrence Convention Center, 304

**Sponsored by:** Diversity & Inclusion

**(754) DIFREX: Nexgen Innovative Technology and Software Solutions, including GRM™ General Reactor Model, for Existing and New Reactor Systems**  
**Monday, Oct 29, 1:45 PM**  
David L. Lawrence Convention Center, 326

**(755) DIFREX: Nexgen Innovative Technology and Software Solutions, including GRM™ General Reactor Model, for Existing and New Reactor Systems**  
**Wednesday, Oct 31, 9:45 AM**  
David L. Lawrence Convention Center, 333

**(756) RAPID Manufacturing Institute Open House**  
**Monday, Oct 29, 5:50 PM**  
David L. Lawrence Convention Center, 335

**Sponsored by:** Process Intensification & Modular Chemical Processing

**(757) AVEVA: Benefits of Digitalization and an Intriguing Usecase Involving Process Simulation**  
**Monday, Oct 29, 3:30 PM**  
David L. Lawrence Convention Center, 326

**(758) Process Systems Enterprise: Hands-on Workshop - Digital Design of Robust Formulated Products and their Manufacturing Processes Through Mechanistic Modelling**  
**Wednesday, Oct 31, 8:00 AM**  
Westin Convention Center, Washington

**(759) Process Systems Enterprise: Introduction to ProcessBuilder - How to Create Value for your Research and Business**  
**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, 320

**(760) MAC Eminent Engineers Awards Ceremony**  
**Monday, Oct 29, 5:30 PM**  
David L. Lawrence Convention Center, 325  
*LaRuth McAfee, Chair*  
*Belinda S. Akpa, Co-Chair*  
**Sponsored by:** Minority Affairs Committee (MAC)

**5:30** Introductory Remarks

**5:35 Paper 760a:** MAC Eminent Engineer Award Winner: Dr. Kafui Dzirasa — *Kafui Dzirasa*

**6:00 Paper 760b:** MAC Eminent Engineer Award Winner: Dr. Cynthia Pierre — *Cynthia Pierre*

**6:25 Paper 760c:** William W. Grimes Award for Excellence in Chemical Engineering Award Winner: Dr. Yusuf Adewuyi — *Yusuf G. Adewuyi*

**6:50** Presentation of Awards, Christine B. Seymour, AIChE President

**(761) Workshop on Identifying the Gaps and Opportunities in Graduate Education to Improve Sustainability of the US Chemical Industries**  
**Thursday, Nov 1, 2:30 PM**  
David L. Lawrence Convention Center, 318

*Ignasi Palou-Rivera, Chair*  
*Alexander Orlov, Co-Chair*

**Sponsored by:** Sustainable Engineering Forum

**(762) AVEVA: Getting Started with SimCentral**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 301

**(763) Knovel: Driving Digital Transformation in Chemistry & Advanced Materials Industry through Decision Support Information Solutions with an Overview of AIChE's Knovel subscription**  
**Monday, Oct 29, 4:45 PM**  
David L. Lawrence Convention Center, 328

**(765) Order of the Engineer Sunday, Oct 28, 5:00 PM**  
David L. Lawrence Convention Center, 306

*Darlene Schuster, Co-Chair*  
*Deborah Grubbe, PE, Co-Chair*  
*Anthony Fregosi, Co-Chair*

**Sponsored by:** Licensing and Professional Development Committee

**(766) ANSYS Inc.: Stay informed-Simulation and analysis software for Chemical and Process Engineering**  
**Wednesday, Oct 31, 8:00 AM**  
David L. Lawrence Convention Center, 328

**(767) Siemens PLM Software: Advanced Simulation (CFD & DEM) to Solve Challenges in the Process Industry**  
**Wednesday, Oct 31, 12:30 PM**  
David L. Lawrence Convention Center, 336

**(768) Innovatia: Bridging the Gap between Engineering and Operations: Work as designed vs. Work as performed**  
**Tuesday, Oct 30, 3:30 PM**  
David L. Lawrence Convention Center, 332

**(769) Innovatia: The Digital Workplace at the Front Line and Where to Begin: Beyond the Digital Twin**  
**Wednesday, Oct 31, 3:30 PM**  
David L. Lawrence Convention Center, 336

**(770) Rockwell Automation: Process Safety – The Lifecycle Explained**  
**Monday, Oct 29, 12:30 PM**  
David L. Lawrence Convention Center, 332



Information as of September 25, 2018.  
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### KEYNOTE SPEAKERS

- Elhanan Borenstein, *University of Washington*
- Pamela Silver, *Harvard Medical School*

### INVITED SPEAKERS

- Cynthia Collins, *Rensselaer Polytechnic Institute*
- Arolyn Conwill, *Massachusetts Institute of Technology*
- Claire Duvallet, *Massachusetts Institute of Technology*
- Almut Heinken, *University of Luxembourg*
- Tami Lieberman, *Massachusetts Institute of Technology*
- Michelle O'Malley, *University of California Santa Barbara*
- Paul Miller, *Synlogic*
- Harris Wang, *Columbia University*

### PANELISTS

- Vanni Bucci, *University of Massachusetts Dartmouth*
- Timothy Lu, *Massachusetts Institute of Technology*
- Costas Maranas, *Pennsylvania State University*
- Bernat Olle, *Vedanta Biosciences*
- Ophelia Venturelli, *University of Wisconsin-Madison*

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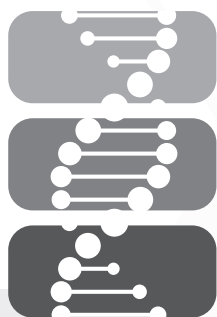
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New Vistas on Shale

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To pay lasting tribute to the late John C. Chen, the Carl R. Anderson Professor Emeritus of Chemical Engineering at Lehigh University and AIChE® President in 2006, the AIChE Foundation has established an endowment fund in his memory to support the leadership development of young professional chemical engineers.

## Thank You to the Founding Donors

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TUESDAY, DECEMBER 11

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Funds raised at this year's Gala will underwrite the expansion of women's leadership programs, improve pre-college STEM education for girls and advance retention programs for women engineering undergraduates, graduate students, and young professionals.

For further information, please contact Donnie Manetta at  
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# The Minority Affairs Committee (MAC)

Celebrates the 2018 Eminent Chemical Engineers and the William W. Grimes Award Winner for Excellence in Chemical Engineering

Monday, October 29 • 5:30 PM - 7:00 PM • David L. Lawrence Convention Center • Room: 325



DIVERSITY & INCLUSION

## Eminent Chemical Engineers Award

MAC's highest award and recognizes outstanding achievements from a professional in a traditional chemical engineering position or from a chemical engineer making significant contributions in a non-traditional profession.



**Kafui Dzirasa, MD, PhD**

K. Ranga Rama Krishnan Endowed Associate Professor  
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**Cynthia Pierre, PhD**

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MAC presents this award in honor of William W. Grimes, the first African-American Fellow of AIChE. The award recognizes a chemical engineer's outstanding achievements as a distinguished role model for minorities.



**Dr. Yusuf G. Adewuyi**

Professor  
North Carolina A&T State University



Promotes activities that will encourage the education and training of minorities in engineering and related disciplines.

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# CRISPR TECHNOLOGIES CONFERENCE

December 10-12, 2018  
Bahia Resort Hotel | San Diego, CA

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This conference will bring together leaders and trainees from the cutting edge of CRISPR technologies and their application to genome editing and beyond. Academic, clinical, and industrial researchers are invited to share their recent discoveries to progress the field in CRISPR science and engineering.

Visit [www.aiche.org/crispr](http://www.aiche.org/crispr) for additional information, including session topics and program.

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## KEYNOTE SPEAKER

- Fyodor Urnov, *Altius Institute for Biomedical Sciences*

## INVITED SPEAKERS

- Omar Akbari, *University of California, San Diego*
- Chase Beisel, *Helmholtz Institute*
- Albert Cheng, *Jackson Laboratory*
- Wei Leong Chew, *Genome Institute of Singapore*
- Mo Ebrahimkhani, *Arizona State University/Mayo Clinic*
- Charles Gersbach, *Duke University*
- Patrick Hsu, *Salk Institute for Biological Studies*
- Yinan Kan, *eGenesis*
- Alexis Komor, *University of California, San Diego*
- Prashant Mali, *University of California, San Diego*
- Megan Palmer, *Stanford University*
- Shengdar Tsai, *St. Jude Children's Research Hospital*
- Harris Wang, *Columbia University*
- Yan Zhang, *University of Michigan*
- John Zuris, *Editas Medicine*

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# FOODIE

FOOD INNOVATION AND  
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December 2-4, 2018 • Napa, CA

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Don't miss this exciting inaugural event focusing on emerging technologies for food production, analyzing strategies to connect industry and cuisine, and navigating methods to fit the consumer market.

Hosted by AIChE's Food, Pharmaceutical & Bioengineering Division, FOODIE will bring together leaders in the field of food technology, science and industry to meet the evolving needs of consumers as they relate to ethical, sustainability, quality and safety food issues.

## Keynote Speakers

- ▶ Laura Kliman, *Impossible Foods*
- ▶ Harold Schmitz, *Mars, Incorporated*

## Invited Speakers

- ▶ Mark Burns, *University of Michigan*
- ▶ Richard Hartel, *University of Wisconsin-Madison*
- ▶ Kathiravan Krishnamurthy, *Illinois Institute of Technology*
- ▶ Nicole Rawling, *The Good Food Institute*
- ▶ Leslie Shor, *University of Connecticut*
- ▶ Bryan Tracy, *White Dog Labs*
- ▶ Greg Ziegler, *Pennsylvania State University*

## Novel Food Processing Technologies Panel Discussion

- ▶ Bala Balasubramaniam, *Ohio State University*
- ▶ Kathiravan Krishnamurthy, *Illinois Institute of Technology*
- ▶ Nitin Nitin, *University of California Davis*
- ▶ Zhongli Pan, *University of California Davis*
- ▶ Suresh D. Pillai, *Texas A&M University*

## Chairs

- ▶ David Block, *University of California Davis*
- ▶ Kate Gawel, *Campbell Soup Company*
- ▶ John Kaiser, *Iowa State University*
- ▶ Nitin Nitin, *University of California Davis*

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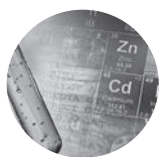
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Chemical  
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- Artificial Intelligence
- Artificial Photosynthesis
- Biomanufacturing for Waste
- Biopolymers
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#### Keynote Speaker

- ★ **Jason Crusan**  
NASA

#### Invited Speakers

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*University of California, Berkeley*
- ★ **Mark Blenner**  
*Clemson University*
- ★ **Frances Houle**  
*Joint Center for Artificial Photosynthesis*
- ★ **Matthew Kanan**  
*Stanford University*
- ★ **Michael Koepke**  
*LanzaTech*
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*Texas A&M University*
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