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Did you know this program book can have another life at the Meeting?

Create a more sustainable future by returning this book when you no longer need it to the registration area where a fellow attendee can enjoy it.

You can also go digital with the AIChEvents app, just download it here:



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.

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2019 ANNUAL MEETING WELCOME



Dear Colleagues:

On behalf of AIChE and its Board of Directors, I welcome you to Orlando and our 2019 Annual Meeting.

This year's meeting spotlights the many ways that chemical engineers are transforming the world through innovation. The program features several new topical conferences that showcase chemical engineers' game-changing contributions, and the diverse workforce that makes it all possible.

With innovation an essential component for achieving the breakthroughs needed to solve global problems, the meeting offers inspiration at a **Meet the Innovators** panel discussion on Tuesday. You'll receive insights from **Rakesh Agrawal** (Purdue Univ.), **Jay Keasling** (Berkeley National Lab), and **Christine Schmidt** (Univ. of Florida).

Another highlight is an expanded **Next-Gen Manufacturing** program. In addition to topics in process intensification, modular manufacturing, and 3D printing, the Next-Gen conference delves into A.I., advanced computation, cybersecurity, and Pharma 4.0. The Next-Gen program is underwritten by the AIChE Foundation through its Doing a World of Good initiative. Other Foundation-supported topical conferences promoting the good works of today's chemical engineers are **Entrepreneurship in Chemical Engineering** and **Food Innovation and Engineering**.

The meeting's featured technical content also includes a new **Applications of Data Science to Molecules and Materials** Topical Conference, with its programming complimented by a panel discussion devoted to **Data Science Education in Chemical Engineering** (Monday). Other topical conferences explore microbes; medicine; fossil, ammonia, and solar energy; green process engineering; sustainable energy; synthetic fuels; sensors; and more.

Some of our profession's brightest lights will shine in our Annual Meeting lectures. This year, AIChE is delighted to unveil two new lectureships:

- Kicking off the meeting on Monday morning is our first Presidential Lecture, presented by Matt Sigelman (Burning Glass Technologies), who will speak about identifying and bridging skills gaps between job seekers and employers.
- On Wednesday, we inaugurate the William R. Schowalter Lecture. The lectureship is endowed by the AIChE Foundation and will be
 delivered by Michael Graham (Univ. of Wisconsin-Madison), whose talk is entitled "Flowing Complex Fluids, from Blood to the Buffer Layer."

Other lectures offer an opportunity to hear from some our profession's most compelling people:

- Monday evening, AIChE's Society for Biological Engineering (SBE) sponsors the **Daniel I. C. Wang Award Lecture**, where **Douglas Clark** (Univ. of California, Berkeley) will explain how to "teach old enzymes new tricks."
- First up on Tuesday morning, **Carlos Rinaldi** (Univ. of Florida) describes the response of magnetic nanoparticles to time-varying magnetic fields in the IACChE's **James Y. Oldshue Lecture**.
- Tuesday morning also features the **Andreas Acrivos Professional Progress Award Lecture**. **Martin Bazant** (MIT) will discuss the "Control of Interfacial Stability in Electrochemical Systems."
- On Tuesday evening, SBE's James E. Bailey Award Lecture will be given by Jens Nielsen (BioInnovation and Chalmers Univ. of Technology), who explores the systems biology of metabolism and its role in the production of biofuels and the diagnosis of diseases.
- Wednesday's John M. Prausnitz AIChE Institute Lecture is by Karen K. Gleason (MIT), who discusses vapor-deposited polymers.

With so much programming in store, download the AIChEvents app to maintain a personal schedule and receive meeting updates on your mobile device. Equally important, be safe and community-conscious. Read the safety information and codes of conduct printed in this book and posted by your hotel.

Also, I encourage you to take full advantage of the networking opportunities you will find at our meeting's exhibits, coffee breaks, poster sessions, and receptions. In particular, take the time to meet some of the many graduate and undergraduate students that attend the conference and encourage them along their career paths.

AIChE offers its gratitude to our meeting sponsor organizations and our Meeting Program Chairs, Venkat Bethanabotla and Richard Dickinson. We also thank the many presenters, authors, session chairs, and volunteers who make all this programming a reality.

To everyone participating at this meeting, I extend my personal thanks. Let's join together to make this Annual Meeting the most rewarding one yet.

Sincerely,

Kimberly Ogden 2019 AIChE President

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MEETING PROGRAM CHAIRS



Wenkat R. Bhethanabotla
Professor, Department of Chemical & Biomedical Engineering
Director, Materials Science and Engineering Program
University of South Florida



MEETING PROGRAM CO-CHAIR
Richard B. Dickinson
Division Director, Chemical, Bioengineering,
Environmental & Transport Systems Division
National Science Foundation
Professor, Department of Chemical Engineering
University of Florida



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2019 ANNUAL MEETING EXHIBITORS

- ACS Publications
- Alliant Insurance Services, Inc.
- Anton Paar
- AON Affinity
- Avant-Garde Materials Simulation
- AVEVA Software LLC
- Biomedical Engineering Society
- Bruker Scientific LLC
- CACHE Corporation
- Cambridge University Press
- · Chemstations, Inc.
- COMSOL
- CRC Press
- De Gruyter
- DigiM Solution
- DIPPR
- EDEM
- Elsevier *
- Equilibar
- ForteBio †
- Frontiers
- Gamry Instruments
- Ghent University
- GRANUTOOLS
- Hanwha TOTAL Petrochemical
- · Heidolph North America
- HIDEN ISOCHEMA LTD
- IKA Works, INC
- Imperial College London
- INFICON
- JSOL Corporation

- Malvern Panalytical
- MDPI
- Molecule Works Inc.
- Nanoscience Instruments
- National Energy Technology Laboratory
- OLI Systems *
- Park Systems
- Parr Instrument Company
- Process Systems Enterprise *
- Rescale
- Royal Society of Chemistry
- SABIC
- Seeq Corporation
- Siemens *
- Software for Chemistry & Materials
- Surface Measurement Systems
- TA Instruments
- TechnipFMC
- Teledyne ISCO †
- Tridiagonal Solutions Inc
- Unchained Labs
- Wiley
- Workrite FRCP
- XPure Systems *
- · XtalPi Inc.
- · Zaiput Flow Technologies
- * Sponsored Technology Workshop Scheduled
- † Featured Exhibitor

Exhibitors as of October 11, 2019.



2019 ANNUAL MEETING INFORMATION

ONSITE INFORMATION & LOGISTICS

Onsite Registration Hours

Hyatt Regency Orlando, Regency Ballroom Foyer *A registration table will be available near the technical sessions taking place on Friday, November 15

| Saturday, November 9 | Noon - 5:00 PM |
|------------------------|--------------------|
| Sunday, November 10 | 8:00 AM - 8:00 PM |
| Monday, November 11 | 7:00 AM - 5:30 PM |
| Tuesday, November 12 | 7:00 AM - 5:30 PM |
| Wednesday, November 13 | 7:30 AM - 5:00 PM |
| Thursday, November 14 | 7:30 AM - 4:30 PM |
| Friday, November 15* | 8:00 AM - 12:00 PM |

2019 AIChE Annual Meeting Exhibit

Hyatt Regency Orlando, Regency Ballroom Foyer

| Sunday, November 10 | 6:30 PM - 7:30 PM |
|----------------------|-------------------|
| Monday, November 11 | 9:30 AM - 5:00 PM |
| Tuesday, November 12 | 9:30 AM - 5:00 PM |



Wireless Internet

We are pleased to offer wireless internet for Meeting attendees throughout the venue.

SSID/Network: AIChEAnnual19
Password: innovate



Professional Headshot Photos

Hyatt Regency Orlando, Regency Ballroom Foyer

New for this year: update your LinkedIn profile picture or resume photo with a complimentary headshot photograph.

Annual Meeting Attendees

| Monday, November 11 | 9:00 AM - 5:00 PM |
|----------------------|-------------------|
| Tuesday, November 12 | 9:00 AM - 5:00 PM |



WIC Family Accommodations Room/ Mother's Room

AIChE has arranged for a mothers' room onsite which will be available for the duration of the Annual Meeting. The room will have a refrigerator and furniture. The room is located behind the registration counters, on the lower level. To gain access, please speak with a customer service representative at the registration area.



Recommended Daycare Services

Below is a list of daycare services recommended by the Hyatt Regency Orlando:

https://www.destinationsitters.com/ www.kidsniteout.com https://supersittersincfl.com/



Shipping & Printing at the Hyatt Regency Orlando

The Hyatt Regency Orlando offers a fully operational Business Center through 11th Hour. The 11th Hour Business Center is available for arranging shipment (both inbound and outbound) and printing services.

| Saturday, November 9 | 7:00 AM - 6:00 PM |
|--|-------------------|
| Sunday, November 10 | 8:00 AM - 6:00 PM |
| Monday, November 11 - Friday, November 15 | 7:00 AM - 8:00 PM |



Lost and Found

For questions and help with Lost and Found please visit the registration area located in the Regency Ballroom Foyer.



The Scavenger Hunt is On!

Collect and find codes throughout the conference to earn points and climb the leaderboard. Be one of 5 lucky winners of a fantastic prize! aiche.org/hunt



Recording & Photography Policy

AlChE 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 AlChE 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. By registering for this conference, you consent to your likeness being used for such purposes without compensation and release AlChE from any liability on account of such usage.



COFFEE BREAKS & REFRESHMENTS

Coffee Breaks

Monday and Tuesday • 10:30 AM - 11:00 AM Hyatt Regency Orlando, Regency Ballroom Fover

Refreshments

Annual Business Meeting

Monday, November 11 • 7:00 AM - 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom H

2019 ANNUAL MEETING INFORMATION

COFFEE BREAKS & REFRESHMENTS (CONTINUED)



2019 Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture

Tuesday, November 12 11:15 AM - 12:15 PM Hyatt Regency Orlando, Plaza International Ballroom H



The National Academies of Sciences, Engineering, and Medicine Town Hall

Wednesday, November 13 8:00 AM - 10:30 AM Hyatt Regency Orlando, Florida Ballroom C



John M. Prausnitz AIChE Institute Lecture

Wednesday, November 13 11:15 AM - 12:15 PM Hyatt Regency Orlando, Plaza International Ballroom H



CONCESSIONS

Regency Ballroom Rotunda Please note times are subject to change.

 Sunday, November 10
 11:00 AM - 5:00 PM

 Monday, November 11
 11:00 AM - 4:00 PM

 Tueday, November 12
 11:00 AM - 4:00 PM



RECEPTIONS

Annual Meeting Opening Reception

Sunday, November 10 • 6:30 PM - 7:30 PM Hyatt Regency Orlando, Regency Ballroom Fover

Enjoy cocktails and food while networking with friends and colleagues.



√ Hyatt Regency Orlando, Regency Ballroom R/S

Monday, November 11 3:30 PM - 5:00 PM
Tuesday, November 12 3:30 PM - 5:00 PM
Wednesday, November 13 3:30 PM - 5:00 PM

TIPS FOR A SUCCESSFUL MEETING



Say hello to everyone.

You might make someone's day.



Introduce yourself to people you don't know.

They may be your next good friends.



Stop and smile.

You will brighten the room considerably.



Be understanding.

Everybody makes mistakes.



Help those with less experience.

We were all novices at some point.



Respect others.

We all have something valuable to contribute.



Value staff and volunteers.

They are here for you.



Be kind

You will never like everybody, but you can be cordial to all.



Enjoy the meeting!

You can have fun while sharing, learning and networking.



We're interested in how science can enhance people's lives. That can mean discovering a new material or working with our customers to apply fresh thinking to the world around us. It can also mean using science to build an exciting career—with the opportunity to explore, exchange ideas, and make a meaningful difference on global challenges.

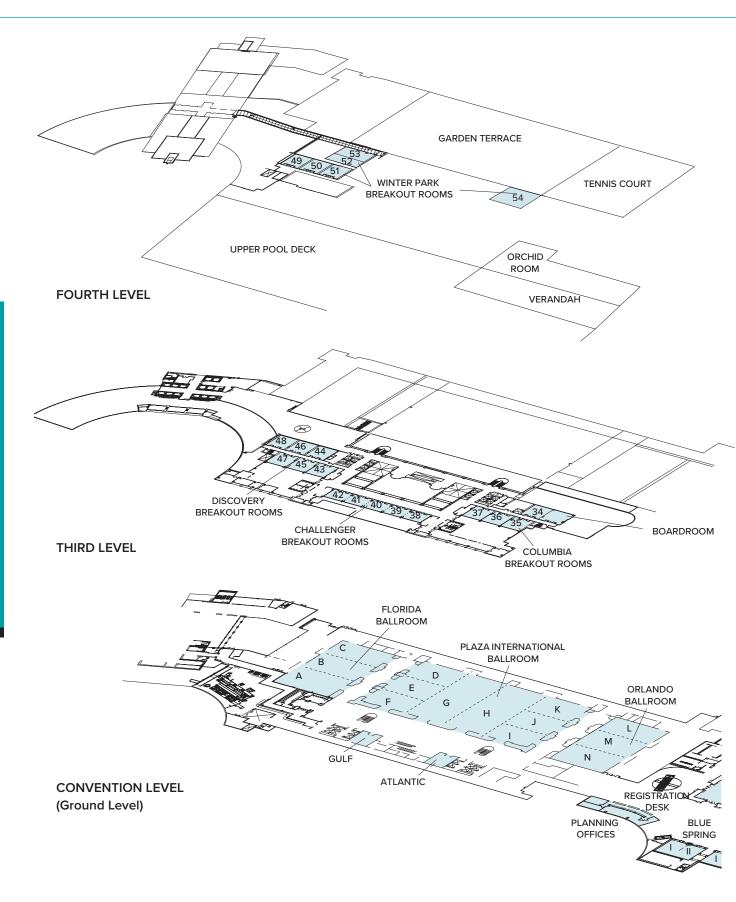
Can you see yourself on the team?



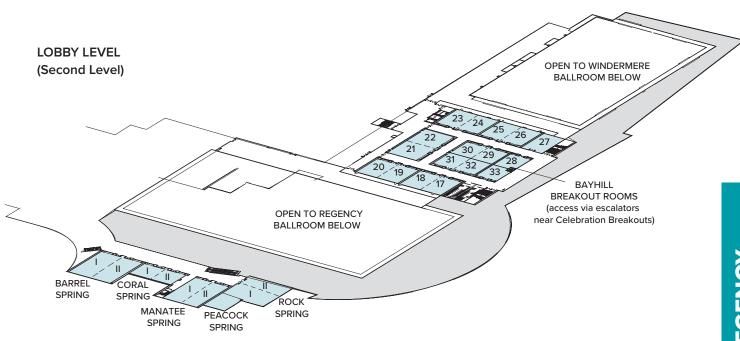
careers.dow.com

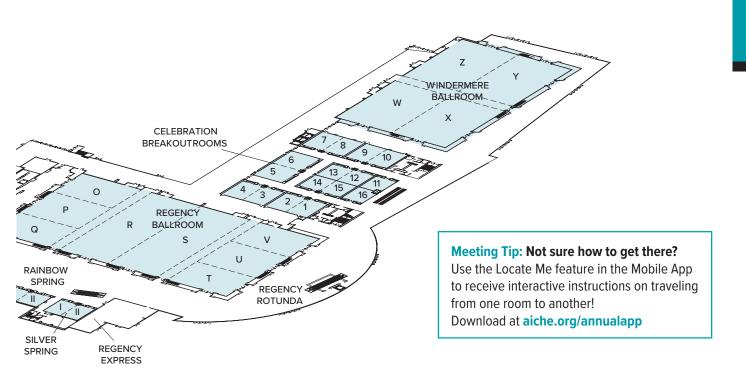
Seek Together[™]

2019 ANNUAL MEETING FLOOR PLAN



2019 ANNUAL MEETING FLOOR PLAN





AIChE Publishing the latest research for the chemical engineering community

AICHE Journal is a high-impact home for quality research publishing on the most exciting technological advances in core areas of chemical engineering and related engineering disciplines.

Driving impact in clinical practice and commercial healthcare products, *Bioengineering & Translational Medicine*, AIChE's fully Gold Open Access journal, 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.

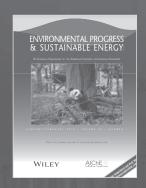
For engineers and scientists, *Environmental Progress* & *Sustainable Energy* reports on critical issues of the environment, providing respected research in this important field.

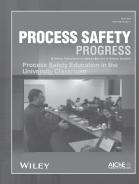
With a clear focus on chemical and hydrocarbon process safety, loss prevention and health, *Process Safety Progress* is widely read by engineering professionals.











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





2019 ANNUAL MEETING PROGRAM GRID KEY

KEY TO SUBJECT AREAS AND TOPICAL CONFERENCES

The full technical program of the 2019 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 6,000 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 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 2019 AIChE Annual Meeting.

04I - Student Chapters Committee Liaison

04K - Department Heads Forum

05A - Professional Development 06 - North American Mixing Forum

04M - Young Faculty Forum

05 - Management Division

| 01A - Thermodynamics and Transport Properties | 07 - Transport and Energy Processes | | | |
|--|--|--|--|--|
| 01C - Interfacial Phenomena | 08 - Materials Engineering and Sciences Division | | | |
| 01D - Transport Processes | 08A - Polymers | | | |
| 01E - Electrochemical Fundamentals | 08B - Biomaterials | | | |
| 01F - High Pressure | 08D - Inorganic Materials | | | |
| 01J - Fluid Mechanics | 08E - Electronics and Photonics | | | |
| 02 - Separations Division | 08F - Composites | | | |
| 02A - Distillation and Absorption | 09 - Environmental Division | | | |
| 02B - Crystallization and Evaporation | 09A - Air | | | |
| 02C - Extractions | 09B - Water | | | |
| 02D - Membrane-Based Separations | 09C - Solid and Hazardous Waste | | | |
| 02E - Adsorption and Ion Exchange | 09D - Process Development | | | |
| 02F - Fluid-Particle Separations | 09F - Fundamentals | | | |
| 02G - Bio Separations | 09G - Sustainability | | | |
| 02H - General Topics and Other Methods | 09H - Climate Change | | | |
| 03 - Particle Technology Forum | 10 - Computing Systems and Technology Division | | | |
| 03A - Particle Production and Characterization | 10A - Systems and Process Design | | | |
| 03B - Fluidization and Fluid-Particle Systems | 10B - Systems and Process Control | | | |
| 03C - Solids Flow, Handling and Processing | 10C - Computers in Operations and Information | | | |
| 03D - Nanoparticles | Processing | | | |
| 03E - Energetics | 10D - Applied Mathematics and Numerical Analysis | | | |
| 04 - Education | 10E - Data and Information Systems | | | |
| 04A - Undergraduate Education | | | | |
| 04B - Graduate Education | - | | | |
| 04G - Professional Development Committee Liaison | - | | | |
| 04H - Career Guidance Committee Liaison | | | | |



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

2019 ANNUAL MEETING PROGRAM GRID KEY

| | Process Development Division I2A - Process Research and Innovation |
|--------|--|
| | 12B - Pilot Plants |
| | I2C - Technology Transfer and Manufacturing |
| | 12E - Process Intensification & Microprocess Engineering |
| | I2G - Product Design |
| 14 - 1 | Nuclear Engineering Division |
| 15 - I | ood, Pharmaceutical & Bioengineering Division |
| • | I5A - Food |
| | 15B - Pharmaceuticals |
| | ISC - Bioengineering |
| | I5D - Engineering Fundamentals in Life Science |
| 16 - I | Fuels and Petrochemicals Division |
| 17 - F | orest and Plant Bioproducts Division |
| 18 - I | iaison Functions |
| | I8A - Miscellaneous |
| | 18B - Public Affairs and Information Committee (PAIC) |
| | ISC - Young Professionals Committee (YPC) |
| | I8D - Publication Committee |
| | I8E - Awards Committee |
| | I8G - Societal Impact Operating Council (SIOC) |
| | I8H - Licensing and Professional Development Committee |
| | 8I - Minority Affairs Committee (MAC) |
| | I8J - Research and New Technology Committee (RANTC) |
| | ISL - International Committee |
| | I8M - Women in Chemical Engineering Committee (WIC) |
| | 180 - Design Institute for Physical Properties (DIPPR) |
| | I8P - Climate Solutions |
| | Catalysis and Reaction Engineering Division |
| | Computational Molecular Science and Engineering Forum |
| 22 - | Nanoscale Science and Engineering Forum |
| | 22A - Carbon Nanomaterials |
| | 22B - Bionanotechnology |
| | 22C - Nanomaterials for Energy Applications |

23 - Sustainable Engineering Forum

23B - Sustainable Biorefineries 23C - Sustainable Energy

23A - Sustainability Science and Engineering

- 24 Chemical Engineering & the Law Forum
- 25 Upstream Engineering and Flow Assurance Forum
- 26 Pharmaceutical Discovery, Development and Manufacturing Forum
- T1 Meet the Faculty and Post-Doc Candidates Poster Session Sponsored by the Education Division
- T2 Entrepreneurship in Chemical Engineering Sponsored by CIEE
- T3 Applications of Data Science to Molecules and Materials
- T4 Concentrated Solar Energy for Power Generation and Chemical Processing
- **T5 Center for Hydrogen Safety**
- **T6 Next-Gen Manufacturing**
 - T6A Next-Gen Manufacturing
 - T6B Process Intensification & Modular Chemical Processing
 - T6C 3D Printing
- **T7 Regenerative Engineering Society**
- **T8 Microbes at Biomedical Interfaces**
- **T9 Sensors**
- **TB Food Innovation and Engineering**
- **TC Engineering for Inclusion**
- **TD Ammonia Energy**
- TE Advances in Fossil Energy R&D
- **TF Chemical Engineers in Medicine**
- TG Innovations of Green Process Engineering for Sustainable Energy and Environment
- **TH Synthetic & Renewable Fuels**
- **TJ Waste Plastics**

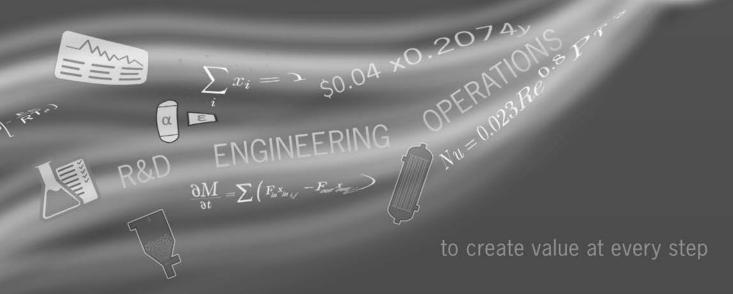
An up-to-date program is available at aiche.org/annual or on the AlChEvents app.



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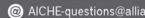
The AIChE Professional Liability (E&O) Insurance Program for Chemical Professionals

Coverage Highlights

- Professional Liability insurance coverage and defense of even frivolous claims
- Coverage for chemical engineers, business owners, and part-time consultants
- Custom coverage for your risk at very competitive rates
- Underwritten by certain underwriters at Lloyd's of London, an "A+" rated carrier
- Administered by Alliant Insurance Services, a proven partner to chemical engineering industries
- Cyber Liability Sublimit (\$500,000) at no additional premium

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"Doing now what patients need next"

AN OPPORTUNITY FOR GROWTH

Our paid internships offer inspiring opportunities for undergraduate and graduate level students to complement their university curriculum with relevant, hands-on experience.

Interns work side-by-side with some of the most talented people in the biotechnology industry. Internships exist in Research, Development, Manufacturing and Engineering, Commercial, Finance, HR, and other corporate business areas. Internships vary in duration, ranging from a minimum of 10 weeks to 12 months, depending on the project requirements.

Summer opportunities will be posted on our careers site December-February. Interviews and selection continue through March.

To view open positions, visit gene.com/careers and search through the Interns/Postdocs Job Type filter.

Genentech's Intern Program, recognized as one of the industry's best, provides students with a chance to experience the biotechnology industry while gaining experience related to their degree. Our program offers unparalleled learning and networking opportunities throughout the company, including the ability to contribute to meaningful projects and interact and work side-by-side with biotech industry experts.

Genentech hires over 500 interns annually across all areas of the business. We provide paid internship opportunities coupled with a flexible and diverse work environment. All interns receive a housing

Our internship positions are located at our headquarters in South San Francisco, CA, and our locations in Vacaville, CA, Oceanside, CA, and Hillsboro, OR.

PROGRAM HIGHLIGHTS

- Opportunity to work on challenging business-critical projects
- Presentation of end-of-summer project findings to senior management
- Networking, career development panels, and speaker series
- Social events
- Eligible Interns will have opportunities to be considered for full-time positions with Genentech

ELIGIBILITY

- We hire Interns at all degree levels: BS, MS, PharmD, and Ph.D.
- Applicants must have completed at least one year of university to be considered for an internship.
- We accept applicants from international students, though visa sponsorship support varies by position and department.

Recent graduates may also apply for internships. You must be within two years of your last degree attained.

@ gene.com/careers

Genentech

REGULATIONS + SAFETY INFORMATION



A NOTE ON PHOTOGRAPHY AND VIDEOGRAPHY FROM THE MEETING ORGANIZERS



Recording & Photography Policy

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 this event is the property of the presenters and the firms where they work. **Recording of sessions or taking photos of slides is strictly prohibited.**

General Photography Notice Sessions and events at the me



Sessions and events at the meeting are being photographed by a professional photographer. These photos will be used to illustrate articles in CEP Chemical Engineering Progress® Magazine, on the AlChE website and in promotional materials for future Meetings. By registering for this conference, you consent to your likeness being used for such purposes without compensation and release AlChE from any liability on account of such usage.

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, get on or off an escalator, walk in a crowd, or make 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.

Please note that all technical sessions take place in the Hyatt Regency Orlando.

| Day | Time | Session # | Session Title | Room |
|-----------|----------|-----------|--|-----------------------------------|
| Monday | 8:00 AM | 63 | Development of Intermolecular Potential Models | Silver Spring I/II |
| Monday | 8:00 AM | 73 | Faculty Candidates in CoMSEF/Area 1a | Peacock Spring |
| Monday | 12:30 PM | 162 | Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks) | Silver Spring I/II |
| Monday | 12:30 PM | 169 | Thermodynamic and Transport Properties Under Pressure I* | Plaza International Ballroom K |
| Monday | 3:30 PM | 204 | Effects of Confinement on Molecular Properties | Rainbow Spring I/II |
| Monday | 3:30 PM | 230 | Thermodynamic and Transport Properties Under Pressure II* | Plaza International Ballroom K |
| Monday | 3:30 PM | 231 | Thermodynamics of Biomolecular Folding and Assembly | Silver Spring I/II |
| Tuesday | 8:00 AM | 247 | Applications of Molecular Modeling to Study Interfacial Phenomena II* | Rock Spring I/II |
| Tuesday | 8:00 AM | 256 | Computational Studies of Self-Assembly | Silver Spring I/II |
| Tuesday | 12:30 PM | 364 | Thermophysical Properties and Phase Behavior | Silver Spring I/II |
| Tuesday | 3:30 PM | 382 | Poster Session: Thermodynamics and Transport Properties (Area 1A) | Regency Ballroom R/S |
| Wednesday | 8:00 AM | 477 | Nucleation and Growth I* | Manatee Spring I |
| Wednesday | 8:00 AM | 480 | Properties and Phase Equilibria for Fuels and Petrochemicals I* | Challenger 38/39 |
| Wednesday | 8:00 AM | 482 | Recent Advances in Molecular Simulation Methods II* | Rock Spring I/II |
| Wednesday | 8:00 AM | 490 | Thermophysical Properties: Complex Systems | Silver Spring I/II |
| Wednesday | 12:30 PM | 544 | Practical Applications of Computational Chemistry and Molecular Simulation I* | Rock Spring I/II |
| Wednesday | 12:30 PM | 547 | Properties and Phase Equilibria for Fuels and Petrochemicals II* | Challenger 38/39 |
| Wednesday | 12:30 PM | 553 | Thermophysical Properties: Polar Compounds and Self-Assembly | Silver Spring I/II |
| Wednesday | 3:30 PM | 590 | Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction | Silver Spring I/II |
| Thursday | 8:00 AM | 643 | Ionic Liquids: Properties and Thermodynamics* | Regency Ballroom Q |
| Thursday | 8:00 AM | 648 | Molecular Simulation and Modeling of Complex Molecules | Peacock Spring |
| Thursday | 8:00 AM | 664 | Thermodynamics Needs of the Chemical Industry | Silver Spring I/II |
| Thursday | 12:30 PM | 690 | Gas Hydrates Science and Engineering | Peacock Spring |
| Thursday | 12:30 PM | 694 | Ionic Liquids: Novel Separation and Reaction Processes* | Regency Ballroom Q |
| Thursday | 12:30 PM | 702 | New Frontiers of Molecular Thermodynamics (Invited Talks) | Silver Spring I/II |
| Thursday | 12:30 PM | 704 | Practical Applications of Computational Chemistry and Molecular Simulation II* | Rock Spring I/II |
| Thursday | 3:30 PM | 728 | Gas Hydrates Science and Engineering: Applications | Peacock Spring |
| Thursday | 3:30 PM | 746 | Thermodynamics at the Nanoscale | Silver Spring I/II |
| Thursday | 3:30 PM | 747 | Thermodynamics of Polymers* | Celebration 12/13 |
| Friday | 8:00 AM | 757 | Modeling of Lipid Membranes and Membrane Proteins | Coral Spring I/II |
| Friday | 12:30 PM | 764 | Inverse Design of Soft Materials | Manatee Spring I |
| Friday | 12:30 PM | 770 | Thermophysical Properties of Biological Systems | Coral Spring I/II |

^{*} This session is co-sponsored by one or more programming groups

| 01C - Interfa | O1C - Interfacial Phenomena | | | | |
|---------------|-----------------------------|-----------|---|-----------------------------------|--|
| Day | Time | Session # | Session Title | Room | |
| Sunday | 3:30 PM | 9 | Active Colloidal Systems | Plaza International Ballroom J | |
| Sunday | 3:30 PM | 16 | Biomolecules at Interfaces I | Plaza International Ballroom K | |
| Monday | 8:00 AM | 56 | Biomolecules at Interfaces II | Plaza International Ballroom K | |
| Monday | 8:00 AM | 78 | Fundamentals of Interfacial Phenomena I | Plaza International Ballroom J | |
| Monday | 8:00 AM | 95 | Solid-Liquid Interfaces | Orlando Ballroom M | |
| Monday | 8:00 AM | 104 | Topical Plenary: Microbial Interactions with Biomaterials and Host Cells (Invited Talks)* | Celebration 9 | |
| Monday | 12:30 PM | 135 | Emerging Antimicrobial Methods* | Celebration 9 | |
| Monday | 12:30 PM | 144 | Fundamentals of Interfacial Phenomena II | Plaza International Ballroom J | |
| Monday | 3:30 PM | 180 | Poster Session: Interfacial Phenomena (Area 1C) | Orlando Ballroom M | |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research* | Celebration 9 | |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 | |
| Tuesday | 8:00 AM | 247 | Applications of Molecular Modeling to Study Interfacial Phenomena II* | Rock Spring I/II | |
| Tuesday | 8:00 AM | 250 | Area Plenary: Interfacial Phenomena (Invited Talks) | Plaza International Ballroom J | |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 | |
| Tuesday | 12:30 PM | 365 | Tribute to Jacob Israelachvili I (Invited Talks) | Plaza International Ballroom K | |
| Tuesday | 3:30 PM | 400 | Emulsions and Foams | Plaza International Ballroom J | |
| Tuesday | 3:30 PM | 430 | Tribute to Jacob Israelachvili II (Invited Talks) | Plaza International Ballroom K | |
| Wednesday | 8:00 AM | 450 | Colloidal Dispersions | Plaza International Ballroom K | |
| Wednesday | 8:00 AM | 465 | Interfacial Aspects of Oil/Gas Recovery and Remediation | Plaza International Ballroom J | |
| Wednesday | 8:00 AM | 485 | Soft Matter Electrokinetics | Plaza International Ballroom I | |
| Wednesday | 12:30 PM | 534 | Interfacial Phenomena in Non-Aqueous Liquids | Plaza International Ballroom J | |
| Wednesday | 12:30 PM | 535 | Interfacial Transport Phenomena | Plaza International Ballroom K | |
| Wednesday | 3:30 PM | 579 | Directed and Self Assembly of Colloids | Plaza International Ballroom J | |
| Wednesday | 3:30 PM | 580 | Dynamic Processes at Interfaces | Plaza International Ballroom K | |
| Thursday | 8:00 AM | 623 | Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications | Orlando Ballroom N | |
| Thursday | 12:30 PM | 698 | Modeling of Interfacial Systems | Orlando Ballroom N | |
| Thursday | 3:30 PM | 742 | Self-Assembly in Solution | Orlando Ballroom N | |

^{*} This session is co-sponsored by one or more programming groups

| Day | Time | Session # | Session Title | Room |
|---------------|-------------|------------|---|-----------------------------------|
| Monday | 12:30 PM | 135 | Emerging Antimicrobial Methods* | Celebration 9 |
| Tuesday | 12:30 PM | 331 | Fundamental Research in Transport Processes | Plaza International Ballroom I |
| Tuesday | 3:30 PM | 414 | Mathematical Modeling of Transport Processes | Plaza International Ballroom I |
| 01E - Electro | chemical Fu | ndamentals | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 71 | Electrochemistry for Applications in Sustainability | Plaza International Ballroom I |
| Monday | 12:30 PM | 136 | Emerging Applications in Electrochemical Separations (Invited Talks) | Plaza International Ballroom I |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research* | Celebration 9 |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 8:00 AM | 286 | Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* | Florida Ballroom A |
| Tuesday | 8:00 AM | 293 | Technologies for Understanding Microbial Interactions* | Celebration 9 |
| Tuesday | 8:00 AM | 297 | Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks) | Plaza Internationa Ballroom I |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 327 | Electrochemical Fundamentals: Faculty Candidate Session | Plaza International Ballroom J |
| Wednesday | 8:00 AM | 484 | Sensor Development Platforms* | Celebration 10 |
| Wednesday | 12:30 PM | 519 | Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions I | Plaza International Ballroom I |
| Wednesday | 3:30 PM | 581 | Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions II | Plaza International Ballroom I |
| Thursday | 8:00 AM | 644 | Lithium and Beyond: Fundamental Advances in High Performance Batteries I | Plaza International Ballroom I |
| Thursday | 12:30 PM | 696 | Lithium and Beyond: Fundamental Advances in High Performance Batteries II | Plaza International Ballroom I |
| 01F - High Pr | essure | | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 25 | High Pressure Phase Equilibria and Modeling | Orlando Ballroom |
| Monday | 8:00 AM | 84 | Materials Synthesis and Processing with Compressed or Supercritical Fluids | Orlando Ballroom |
| Monday | 12:30 PM | 169 | Thermodynamic and Transport Properties Under Pressure I | Plaza International Ballroom K |
| Monday | 3:30 PM | 230 | Thermodynamic and Transport Properties Under Pressure II | Plaza Internationa Ballroom K |
| Friday | 12:30 PM | 768 | Reactions in Near-Critical and Supercritical Fluids* | Celebration 6 |

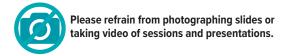


 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

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|----------------|---------------|---------------|--|-----------------------------------|
| Day | Time | Session # | Session Title | Room |
| Monday | 12:30 PM | 123 | Complex Flows and Soft Mechanics (Invited Talks) | Orlando Ballroom L |
| Monday | 3:30 PM | 221 | Poster Session: Fluid Mechanics | Orlando Ballroom M |
| Tuesday | 8:00 AM | 255 | Colloidal Hydrodynamics | Orlando Ballroom L |
| Tuesday | 8:00 AM | 296 | Turbulent and Reactive Flows and Flow Characterization | Orlando Ballroom M |
| Tuesday | 12:30 PM | 334 | Hydrodynamics of Soft and Active Systems | Orlando Ballroom L |
| Tuesday | 12:30 PM | 343 | Interfacial and Nonlinear Flows | Orlando Ballroom M |
| Tuesday | 3:30 PM | 408 | Hydrodynamics of Biological Systems | Orlando Ballroom L |
| Tuesday | 3:30 PM | 416 | Microfluidic and Nanoscale Flows: Separations and Particulates | Orlando Ballroom M |
| Wednesday | 8:00 AM | 469 | Microfluidic and Nanoscale Flows: Multiphase Systems and External Fields | Orlando Ballroom M |
| Wednesday | 8:00 AM | 479 | Particulate and Multiphase Flows: Colloids and Grains | Orlando Ballroom L |
| Wednesday | 12:30 PM | 513 | Complex Fluids | Orlando Ballroom M |
| Wednesday | 12:30 PM | 541 | Particulate and Multiphase Flows: Emulsions and Droplets | Orlando Ballroom L |
| Wednesday | 3:30 PM | 573 | Complex Fluids: Polymers and Macromolecules | Orlando Ballroom M |
| Wednesday | 3:30 PM | 601 | Particulate and Multiphase Flows: Foams and Bubbles | Orlando Ballroom L |
| 02 - Separat | ions Divisio | n | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 8 | 3D Printing Applications in Catalysts, Reactions, and Energy Industry* | Bayhill 28 |
| Monday | 8:00 AM | 69 | Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks) | Manatee Spring II |
| Monday | 12:30 PM | 132 | Division Plenary: Major Separations Challenges (Invited Talks) | Manatee Spring II |
| Monday | 12:30 PM | 136 | Emerging Applications in Electrochemical Separations (Invited Talks)* | Plaza International Ballroom I |
| Tuesday | 12:30 PM | 341 | In Recognition of the 50th Anniversary of ExxonMobil Corporate Strategic Research: SEP (Invited Talks) | Rainbow Spring I/II |
| Tuesday | 3:30 PM | 381 | Poster Session: Separations Division | Regency Ballroom R/S |
| Thursday | 8:00 AM | 643 | Ionic Liquids: Properties and Thermodynamics* | Regency Ballroom Q |
| Thursday | 12:30 PM | 694 | Ionic Liquids: Novel Separation and Reaction Processes* | Regency Ballroom Q |
| 02A - Distilla | tion and Ab | sorption | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 12:30 PM | 131 | Distillation Processes Fundamentals, Developments, and Applications | Barrel Spring II |
| Monday | 3:30 PM | 202 | Distillation: Recent Developments in Advanced Techniques and Process Intensification | Barrel Spring II |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G |
| Tuesday | 12:30 PM | 358 | Refining and Petrochemical Plant Modelling and Operations Improvements* | Challenger 38/39 |
| 02B - Crysta | llization and | l Evaporation | 1 | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 42 | Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond | Coral Spring I/II |
| Monday | 12:30 PM | 125 | Continuous Crystallization Processes | Coral Spring I/II |
| Monday | 3:30 PM | 198 | Crystallization of Pharmaceutical and Biological Molecules | Coral Spring I/II |
| | 1 | 1 | , | |

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| Tuesday | 8:00 AM | 287 | PAT and Process Monitoring in Crystallization Development and Manufacturing | Manatee Spring I |
|---------------|------------|-------------|--|-------------------|
| Tuesday | 12:30 PM | 349 | Modeling and Control of Crystallization II | Coral Spring I/II |
| Wednesday | 8:00 AM | 477 | Nucleation and Growth I | Manatee Spring I |
| Wednesday | 3:30 PM | 599 | Nucleation and Growth II | Manatee Spring I |
| Wednesday | 3:30 PM | 600 | Particle Engineering and Crystallization in Materials Science* | Celebration 6 |
| Thursday | 8:00 AM | 651 | Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions | Coral Spring I/II |
| 02C - Extract | tions | | | |
| Day | Time | Session # | Session Title | Room |
| Wednesday | 12:30 PM | 517 | Developments in Extractive Separations: Solvents | Barrel Spring II |
| Wednesday | 3:30 PM | 578 | Developments in Extractive Separations: Processes | Barrel Spring II |
| 02D - Memb | rane-Based | Separations | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 20 | Charged Polymers for Membrane-Based Water and Energy Applications | Barrel Spring II |
| Sunday | 3:30 PM | 27 | Membranes for CO ₂ Capture | Barrel Spring I |
| Monday | 12:30 PM | 146 | In Honor of Ruth Baltus I (Invited Talks) | Barrel Spring I |
| Monday | 3:30 PM | 213 | In Honor of Ruth Baltus II (Invited Talks) | Barrel Spring I |
| Tuesday | 8:00 AM | 278 | Membrane Formation | Barrel Spring I |
| Tuesday | 12:30 PM | 314 | Bioinspired Membranes and Membrane Processes | Barrel Spring I |
| Wednesday | 8:00 AM | 462 | Highly Selective Separations with Membranes I | Barrel Spring I |
| Wednesday | 12:30 PM | 518 | Diffusion in Polymers* | Celebration 5 |
| Wednesday | 12:30 PM | 531 | Highly Selective Separations with Membranes II | Barrel Spring I |
| Wednesday | 3:30 PM | 569 | Antifouling Membranes for Water Purification | Peacock Spring |
| Wednesday | 3:30 PM | 586 | Industry Perspectives on Membrane Separations (Invited Talks) | Barrel Spring I |
| Thursday | 8:00 AM | 646 | Membrane-Based Organic Solvent Separations I | Barrel Spring II |
| Thursday | 8:00 AM | 665 | Water Treatment, Desalination, and Reuse I | Barrel Spring I |
| Thursday | 12:30 PM | 697 | Mixed-Matrix Materials for Gas Separation | Coral Spring I/II |
| Thursday | 12:30 PM | 709 | Surface Engineered and Responsive Membranes | Barrel Spring II |
| Thursday | 12:30 PM | 714 | Water Treatment, Desalination, and Reuse II | Barrel Spring I |
| Thursday | 3:30 PM | 716 | Advanced Inorganic Materials for Membrane Gas Separation | Coral Spring I/II |
| Thursday | 3:30 PM | 730 | Membrane-Based Organic Solvent Separations II | Barrel Spring II |
| Thursday | 3:30 PM | 731 | Membrane Modeling and Simulation I | Manatee Spring I |
| Thursday | 3:30 PM | 748 | Water Treatment, Desalination, and Reuse III | Barrel Spring I |
| Friday | 8:00 AM | 750 | Advanced Polymeric Membranes for Gas Separation | Barrel Spring I |
| Friday | 8:00 AM | 756 | Membrane Modeling and Simulation II | Barrel Spring II |



 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| Day | Time | Session # | Session Title | Room |
|---------------|---------------|--------------|---|-----------------------------------|
| Day | Time | 3C33IOII # | | Room |
| Monday | 12:30 PM | 113 | Area Plenary: Adsorption and Ion Exchange - In Honor of Celio Cavalcante (Invited Talks) | Manatee Spring I |
| Monday | 3:30 PM | 191 | Adsorption Applications for Sustainable Energy and Chemicals | Manatee Spring II |
| Monday | 3:30 PM | 223 | PSA/TSA | Manatee Spring I |
| Tuesday | 8:00 AM | 288 | Plenary Session: Chromatographic Separations and SMB - In Honor of Linda Wang (Invited Talks) | Manatee Spring II |
| Tuesday | 12:30 PM | 350 | Molecular Simulation of Adsorption I | Manatee Spring II |
| Tuesday | 12:30 PM | 359 | Structured Adsorbents: Beyond Pellets and Beads | Manatee Spring I |
| Tuesday | 3:30 PM | 377 | Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange | Regency Ballroom R/S |
| Wednesday | 8:00 AM | 454 | Diffusion, Transport, and Dynamics in Adsorption Systems | Manatee Spring II |
| Wednesday | 8:00 AM | 483 | Scale-up, Revamp, and Industrial Applications of Adsorption | Regency Ballroom U |
| Wednesday | 12:30 PM | 514 | CO ₂ Capture By Adsorption | Manatee Spring II |
| Wednesday | 12:30 PM | 527 | Fundamentals and Applications of Adsorption and Ion Exchange | Florida Ballroom C |
| Wednesday | 3:30 PM | 583 | Experimental Methods in Adsorption | Blue Spring I/II |
| Wednesday | 3:30 PM | 592 | Molecular Simulation of Adsorption II | Manatee Spring II |
| Thursday | 8:00 AM | 619 | Adsorbent Materials | Manatee Spring I |
| Thursday | 8:00 AM | 631 | Characterization of Adsorbent Materials | Manatee Spring II |
| Thursday | 12:30 PM | 667 | Adsorbent Materials for Sustainable Energy and Chemicals | Manatee Spring I |
| Thursday | 12:30 PM | 668 | Adsorbent Materials: MOFs | Manatee Spring II |
| 02F - Fluid-P | article Sepa | rations | | |
| Day | Time | Session # | Session Title | Room |
| Wednesday | 8:00 AM | 440 | Advances in Fluid Particle Separations | Coral Spring I/II |
| Wednesday | 12:30 PM | 524 | Fluid Particle Separation in Energy and Environmental Systems | Coral Spring I/II |
| Wednesday | 3:30 PM | 610 | Solid-Fluid Separations in Oil & Gas Production and Refining Processes | Coral Spring I/II |
| 02G - Bio Se | parations | | | |
| Day | Time | Session # | Session Title | Room |
| Tuesday | 8:00 AM | 239 | Advances in Bioseparations | Barrel Spring II |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G |
| Tuesday | 12:30 PM | 320 | Chromatography Techniques for Bioprocessing | Barrel Spring II |
| Tuesday | 3:30 PM | 374 | Poster Session: Bioseparations | Regency Ballroom R/S |
| Wednesday | 8:00 AM | 468 | Membranes for Bioseparations | Barrel Spring II |
| 02H - Genera | al Topics and | d Other Meth | nods | |
| Day | Time | Session # | Session Title | Room |
| Tuesday | 3:30 PM | 378 | Poster Session: General Topics on Separations | Regency Ballroom R/S |

^{*} This session is co-sponsored by one or more programming groups

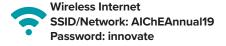
| 03 - Particle | Technology | Forum | | |
|---------------|--------------|--------------|--|----------------------|
| Day | Time | Session # | Session Title | Room |
| Tuesday | 8:00 AM | 287 | PAT and Process Monitoring in Crystallization Development and Manufacturing* | Manatee Spring I |
| Tuesday | 12:30 PM | 340 | Innovations in Particle Engineering: From Amorphous Solid Dispersions to New Processing* | Celebration 7 |
| Tuesday | 3:30 PM | 380 | Poster Session: Particle Technology Forum | Regency Ballroom R/S |
| Wednesday | 8:00 AM | 440 | Advances in Fluid Particle Separations* | Coral Spring I/II |
| Wednesday | 8:00 AM | 492 | Understanding Powder Processing via Materials Science* | Celebration 14 |
| Wednesday | 12:30 PM | 496 | 3D Printing in Pharmaceutical and Health Industry* | Bayhill 28 |
| Wednesday | 12:30 PM | 540 | Particle Technology Awards Lectures (Invited Talks) | Bayhill 19 |
| Wednesday | 3:30 PM | 567 | 3D Printing Fundamental and Applications* | Bayhill 28 |
| Wednesday | 3:30 PM | 600 | Particle Engineering and Crystallization in Materials Science* | Celebration 6 |
| Wednesday | 3:30 PM | 603 | Polymers in Additive Manufacturing* | Bayhill 27 |
| Thursday | 8:00 AM | 651 | Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions* | Coral Spring I/II |
| 03A - Particl | e Productio | n and Charac | cterization | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 42 | Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond* | Coral Spring I/II |
| Monday | 8:00 AM | 49 | Agglomeration and Granulation Processes | Bayhill 20 |
| Monday | 12:30 PM | 120 | Characterization of Engineered Particles and Nanostructured Particulate Systems | Bayhill 20 |
| Monday | 3:30 PM | 220 | Particle Breakage and Comminution Processes | Bayhill 20 |
| Tuesday | 8:00 AM | 262 | Dynamics and Modeling of Particles, Crystals and Agglomerate Formation | Bayhill 21 |
| Tuesday | 12:30 PM | 340 | Innovations in Particle Engineering: From Amorphous Solid Dispersions to New Processing* | Celebration 7 |
| Tuesday | 12:30 PM | 356 | Population Balance Modeling for Particle Formation Processes: Nucleation, Aggregation and Breakage Kernels | Bayhill 20 |
| Wednesday | 8:00 AM | 492 | Understanding Powder Processing via Materials Science* | Celebration 14 |
| Wednesday | 3:30 PM | 600 | Particle Engineering and Crystallization in Materials Science* | Celebration 6 |
| Thursday | 8:00 AM | 633 | Control and Optimization of Particle and Solid Production | Bayhill 20 |
| Thursday | 3:30 PM | 738 | Particle Engineering and Design for Product Value Enhancement | Bayhill 20 |
| 03B - Fluidiz | ation and Fl | uid-Particle | Systems | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 77 | Fundamentals of Fluidization | Bayhill 19 |
| Monday | 12:30 PM | 140 | Experimental Investigation of Fluidization Processes | Bayhill 19 |
| Monday | 3:30 PM | 228 | Session in Honor of Prof. Atsushi Tsutsumi's Accomplishments | Bayhill 19 |
| Tuesday | 8:00 AM | 292 | Special Session: Celebrating Career Accomplishments of Fred Zenz | Bayhill 19 |
| Tuesday | 12:30 PM | 336 | Industrial Application of Computational and Numerical Approaches to Particle Flow | Bayhill 19 |
| Wednesday | 3:30 PM | 572 | Circulating Fluidized Beds | Bayhill 19 |
| Thursday | 8:00 AM | 647 | Modeling Approaches and Applications in Fluidization Fundamentals | Bayhill 19 |
| Thursday | 12:30 PM | 688 | Fluidization and Fluid-Particle Systems for Energy and Environmental Applications | Bayhill 19 |
| Thursday | 3:30 PM | 732 | Modeling of Fluidization Processes | Bayhill 19 |

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| 03C - Solids Flow, Handling and Processing | | | | | |
|--|---------------------|------------|--|----------------------------------|--|
| Day | Time | Session # | Session Title | Room | |
| Monday | 8:00 AM | 96 | Solids Handling and Processing in Particulate Systems | Bayhill 21 | |
| Monday | 12:30 PM | 133 | Dynamics and Modeling of Particulate Systems: Discrete and Continuum | Bayhill 21 | |
| Monday | 3:30 PM | 203 | Dust Explosions and Process Safety in Solids Processing | Bayhill 21 | |
| Tuesday | 12:30 PM | 348 | Mixing and Segregation of Particulates | Bayhill 21 | |
| Tuesday | 3:30 PM | 397 | Conversion of Solid Wastes to Energy and/or Product* | Regency Ballroom Q | |
| Wednesday | 8:00 AM | 456 | Dynamics and Modeling of Particulate Systems: Applications | Bayhill 21 | |
| Thursday | 8:00 AM | 652 | Particle Separations (Solid/Solid, Solid/Liquid, Solid/Gas) | Bayhill 21 | |
| Thursday | 12:30 PM | 680 | Characterization and Measurement in Powder Processing | Bayhill 21 | |
| Thursday | 12:30 PM | 703 | Particle Technology in Product Design | Bayhill 20 | |
| Thursday | 3:30 PM | 743 | Solids Handling: Characterization and Heat Transfer | Bayhill 21 | |
| 03D - Nanop | articles | | | | |
| Day | Time | Session # | Session Title | Room | |
| Tuesday | 8:00 AM | 264 | Functional Nanoparticles | Bayhill 20 | |
| Wednesday | 8:00 AM | 476 | Novel Nanoparticles and Nanostructured Materials for Catalysis | Bayhill 19 | |
| Wednesday | 12:30 PM | 528 | Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles | Bayhill 20 | |
| Wednesday | 3:30 PM | 598 | Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications | Bayhill 20 | |
| 03E - Energe | tics | | | | |
| Day | Time | Session # | Session Title | Room | |
| Wednesday | 8:00 AM | 458 | Energetic Materials: Engineered Particles and Interfaces | Bayhill 20 | |
| Wednesday | 12:30 PM | 501 | Advances in Processing and Handling of Energetic Materials | Bayhill 21 | |
| Wednesday | 3:30 PM | 568 | Additive Manufacturing of Energetics | Bayhill 21 | |
| 04 - Educatio | on | | | | |
| Day | Time | Session # | Session Title | Room | |
| Sunday | 1:00 PM | 6 | Meet the Faculty and Post-Doc Candidates Poster Session* | Regency Ballroom R/S | |
| Sunday | 3:30 PM | 47 | Workshop: Writing Successful Education Proposals | Bayhill 23 | |
| Monday | 8:00 AM | 100 | Student Paper Competition in Sensor Technology I* | Celebration 10 | |
| Monday | 12:30 PM | 130 | Digital Twin (Invited Talks)* | Bayhill 28 | |
| Monday | 12:30 PM | 163 | Student Paper Competition in Sensor Technology II* | Celebration 10 | |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research* | Celebration 9 | |
| Tuesday | 8:00 AM | 261 | DORIC: Supporting Our Students with Disabilities* | Bayhill 31 | |
| Tuesday | 8:00 AM | 273 | In Honor of the 2018 Recipient of the Warren K. Lewis Award (Invited Talks) | Bayhill 22 | |
| Tuesday | 12:30 PM | 326 | Education Division Plenary: Award Winners and Perspectives on 10 Years of the Education Division (Invited Talks) | Bayhill 22 | |
| | | | | | |
| Tuesday | 12:30 PM | 329 | Experiences in Teaching Process Safety I* | Bayhill 17 | |
| | 12:30 PM 3:30 PM | 329 375 | Experiences in Teaching Process Safety I* Poster Session: Chemical Engineering Education | Bayhill 17 Regency Ballroom R/S | |
| Tuesday | | | | , | |
| Tuesday | 3:30 PM | 375 | Poster Session: Chemical Engineering Education | Regency Ballroom R/S | |

^{*} This session is co-sponsored by one or more programming groups

| Monday 8:00 AM 61 Free Forum on Engineering Education: First Year and Sophomore Year Bayhill 23 Monday 8:00 AM 97 Steal this Coursel: Electives and Novel Course Offerings Bayhill 22 Monday 12:30 PM 142 Free Forum on Engineering Education: Junior and Senior Years I Bayhill 23 Monday 3:30 PM 190 ABET Updates and Insights (Invited Talks) Bayhill 22 Monday 3:30 PM 207 Free Forum on Engineering Education: Junior and Senior Years II Bayhill 23 Tuesday 8:00 AM 263 Computing for ChEs: Teaching Programming and Simulation Software Bayhill 29/30 Tuesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 29/30 Wednesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 23 Wednesday 12:30 PM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 585 How We Teach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Day Time Session # Session Title Wonday 12:30 PM 168 Workshop: Effective Teaching for New or Prospective Faculty Rock Spring I/II Monday 12:30 PM 168 Workshop: Effective Teaching for New or Prospective Faculty Rock Spring I/II Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Bayhill 22 DAY Time Session # Session Title Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 Monday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 DAY Time Session # Session Title Room Windermere Ballroom Monday 8:00 AM 98 Student Design Competition Bayhill 29/30 DAY Time Session # Session Title Room Wednesday 8:00 AM 99 Student Paper Competition Bayhill 29/30 DAY Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 DAY Time Session # Session Title Wednesday 8:00 AM 453 Department Heads Forum (Inv | Wednesday | 3:30 PM | 571 | CACHE 50th Anniversary: The Future of Cyber-Assisted Chemical Engineering Education* | Regency Ballroom T |
|--|--------------|--------------|--------------|--|---------------------|
| Monday 8:00 AM 61 Free Forum on Engineering Education: First Year and Sophomore Year Bayhill 23 Monday 8:00 AM 97 Steal this Coursel: Electives and Novel Course Offerings Bayhill 22 Monday 12:30 PM 142 Free Forum on Engineering Education: Junior and Senior Years I Bayhill 23 Monday 3:30 PM 190 ABET Updates and Insights (Invited Talks) Bayhill 22 Monday 3:30 PM 207 Free Forum on Engineering Education: Junior and Senior Years II Bayhill 23 Monday 8:00 AM 263 Computing for ChEs: Teaching Programming and Simulation Software Bayhill 29/30 Tuesday 8:00 AM 263 Computing for ChEs: Teaching Programming and Simulation Software Bayhill 29/30 Wednesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 23 Wednesday 8:00 AM 257 Effective Communication Skills for ChE Bayhill 23 Wednesday 12:30 PM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 585 How We Teach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Bayhill 22 04G - Professional Development Committee Liaison Day Time Session # Session Title Nonday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Rock Spring I/II Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop: Effective Teaching of Prospective Faculty Rock Spring I/II Monday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 04I - Student Chapters Committee Liaison Day Time Session # Session Title Room Windermere Ballroon Monday 3:30 PM 5 Chem-E-Car Competition Bayhill 29/30 04I - Student Chapters Committee Liaison Day Time Session # Session Title Room Wednesday 8:00 AM 98 Student Design Competition Bayhill 29/30 04K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invit | 04A - Under | graduate Ed | ucation | | |
| Monday 8:00 AM 97 Steal this Course!: Electives and Novel Course Offerings Bayhill 22 Monday 12:30 PM 142 Free Forum on Engineering Education: Junior and Senior Years I Bayhill 23 Monday 3:30 PM 190 ABET Updates and Insights (Invited Talks) Bayhill 22 Monday 3:30 PM 207 Free Forum on Engineering Education: Junior and Senior Years II Bayhill 23 Tuesday 8:00 AM 263 Computing for ChEs: Teaching Programming and Simulation Software Bayhill 29/30 Tuesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 23 Wednesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 23 Wednesday 8:00 AM 27 Effective Communication Skills for ChE Bayhill 23 Wednesday 12:30 PM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 585 How We Teach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Bayhill 22 O4G - Professional Development Committee Liaison Day Time Session # Session Title Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Rock Spring I/II Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Rock Spring I/II Monday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 3:30 PM 5 Chem-E-Car Competition Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session Title Nonday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session Title Room Windermere Ballroot Monday 8:00 AM 98 Student Design Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 | Day | Time | Session # | Session Title | Room |
| Monday 12:30 PM 142 Free Forum on Engineering Education: Junior and Senior Years I Bayhill 23 Monday 3:30 PM 190 ABET Updates and Insights (Invited Talks) Bayhill 22 Monday 3:30 PM 207 Free Forum on Engineering Education: Junior and Senior Years II Bayhill 23 Tuesday 8:00 AM 263 Computing for ChEs: Teaching Programming and Simulation Software Bayhill 29/30 Tuesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 23 Wednesday 8:00 AM 457 Effective Communication Skills for ChE Bayhill 23 Wednesday 8:00 AM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 585 How We feach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Bayhill 22 04G- Professional Development Committee Liaison Day Time Session # Session Title Room Sunday 3:30 PM 46 Workshop: Effective Teaching for New or Prospective Faculty Rock Spring I/II Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Bayhill 22 04H - Career Guidance Committee Liaison Day Time Session # Session Title Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 04I - Student Chapters Committee Liaison Day Time Session # Session Title Nonday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 04I - Student Chapters Committee Liaison Day Time Session # Session Title Nonday 8:00 AM 98 Student Design Competition Bayhill 29/30 04K - Department Heads Forum Day Time Session # Session Title Room Day Time Session # Ses | Monday | 8:00 AM | 61 | Free Forum on Engineering Education: First Year and Sophomore Year | Bayhill 23 |
| Monday 3:30 PM 190 ABET Updates and Insights (Invited Talks) Bayhill 22 Monday 3:30 PM 207 Free Forum on Engineering Education: Junior and Senior Years II Bayhill 23 Tuesday 8:00 AM 263 Computing for ChEs: Teaching Programming and Simulation Software Bayhill 29/30 Tuesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 23 Wednesday 8:00 AM 457 Effective Communication Skills for ChE Bayhill 23 Wednesday 12:30 PM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 585 How We Teach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Bayhill 22 O4G - Professional Development Committee Liaison Day Time Session # Session Title Room Sunday 3:30 PM 46 Workshop: Effective Teaching for New or Prospective Faculty Rock Spring I/II Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Bayhill 22 O4H - Career Guidance Committee Liaison Day Time Session # Session Title Nonday 10:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 12:30 PM 59 Session # Session Title Nonday 3:30 PM 217 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session # Session Title Nonday 3:30 PM 5 Chem-E-Car Competition Bayhill 25 Nonday 8:00 AM 98 Student Design Competition Bayhill 25 Nonday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session # Session Title Nonday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Monday | 8:00 AM | 97 | Steal this Course!: Electives and Novel Course Offerings | Bayhill 22 |
| Monday 3:30 PM 207 Free Forum on Engineering Education: Junior and Senior Years II Bayhill 23 Tuesday 8:00 AM 263 Computing for ChEs: Teaching Programming and Simulation Software Bayhill 29/30 Tuesday 8:00 AM 266 How We Teach: Ethics, Teamwork, Leadership, and Professional Skills Bayhill 23 Wednesday 8:00 AM 457 Effective Communication Skills for ChE Bayhill 23 Wednesday 12:30 PM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 585 How We Teach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Bayhill 22 DdG- Professional Development Committee Liaison Day Time Session # Session Title Session # Monday 12:30 PM 168 Workshop: Effective Teaching for New or Prospective Faculty Bayhill 22 DdH - Career Guidance Committee Liaison Day Time Session # Session Title Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 12:30 PM 157 NSF Workshop I: Proposal Writing and Discussions with Program Managers Bayhill 29/30 DdJ - Student Chapters Committee Liaison Day Time Session # Session Title Sunday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 OdJ - Student Chapters Committee Liaison Day Time Session # Session Title Sunday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 OdJ - Student Chapters Committee Liaison Day Time Session # Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 OdK - Department Heads Forum Day Time Session # Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 OdK - Department Heads Forum Day Time Session # Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Bayhill 29/30 OdK - Department Heads Forum Day Time Session # Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Day Time Session | Monday | 12:30 PM | 142 | Free Forum on Engineering Education: Junior and Senior Years I | Bayhill 23 |
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| Wednesday 8:00 AM 457 Effective Communication Skills for ChE Bayhill 23 Wednesday 12:30 PM 550 Teaching Using Desktop Learning Modules and Laboratory Activities Bayhill 23 Wednesday 3:30 PM 585 How We Teach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques O4G - Professional Development Committee Liaison Day Time Session # Session Title Room Sunday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Bayhill 22 O4H - Career Guidance Committee Liaison Day Time Session # Session Title Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 12:30 PM 154 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Bayhill 25 Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 98 Student Paper Competition Bayhill 25 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Tuesday | 8:00 AM | 263 | Computing for ChEs: Teaching Programming and Simulation Software | Bayhill 29/30 |
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| Wednesday 3:30 PM 585 How We Teach: First Year Students Survey Results (Invited Talks) Bayhill 23 Wednesday 3:30 PM 589 LAAARGE Classroom Techniques Bayhill 22 O4G - Professional Development Committee Liaison Day Time Session # Session fitle Sunday 3:30 PM 46 Workshop: Effective Teaching for New or Prospective Faculty Rock Spring I/II Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Bayhill 22 O4H - Career Guidance Committee Liaison Day Time Session # Session Title Room Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 3:30 PM 217 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session Title Room Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Wednesday | 8:00 AM | 457 | Effective Communication Skills for ChE | Bayhill 23 |
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| Day Time Session # Session Title Session # Session Title Room | Wednesday | 3:30 PM | 585 | How We Teach: First Year Students Survey Results (Invited Talks) | Bayhill 23 |
| Session # Session # Session fitle Room | Wednesday | 3:30 PM | 589 | LAAARGE Classroom Techniques | Bayhill 22 |
| Sunday 3:30 PM 46 Workshop: Effective Teaching for New or Prospective Faculty Rock Spring I/II Monday 12:30 PM 168 The Path Less Traveled: Professional Development for Non-Tenure Track Faculty Bayhill 22 04H - Career Guidance Committee Liaison Day Time Session # Session Title Room Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 3:30 PM 217 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 04I - Student Chapters Committee Liaison Day Time Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Windermere Ballroot Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 04K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) DAY Time Session # Session Title Room Wednesday 8:00 AM 5ession # Session Title Room | 04G - Profes | sional Deve | lopment Cor | nmittee Liaison | |
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| Day Time Session # Session Title Room Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 Monday 3:30 PM 217 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Windermere Ballroon Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Sunday | 3:30 PM | 46 | Workshop: Effective Teaching for New or Prospective Faculty | Rock Spring I/II |
| Time Session # Session Title Room Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 3:30 PM 217 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Windermere Ballroon Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Monday | 12:30 PM | 168 | The Path Less Traveled: Professional Development for Non-Tenure Track Faculty | Bayhill 22 |
| Sunday 10:00 AM 4 Workshop: Career Planning for Prospective Faculty Rock Spring I/II Monday 12:30 PM 154 NSF Workshop I: Highlights from CBET Bayhill 29/30 Monday 3:30 PM 217 NSF Workshop II: Proposal Writing and Discussions with Program Managers Bayhill 29/30 O4I - Student Chapters Committee Liaison Day Time Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Windermere Ballroot Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | 04H - Career | Guidance (| Committee Li | aison | |
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| Day Time Session # Session Title Room Sunday 12:30 PM 5 Chem-E-Car Competition Windermere Ballroom Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Day Time Session # Session Title Room Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Monday | 12:30 PM | 154 | NSF Workshop I: Highlights from CBET | Bayhill 29/30 |
| DayTimeSession #Session TitleRoomSunday12:30 PM5Chem-E-Car CompetitionWindermere BallroomMonday8:00 AM98Student Design CompetitionBayhill 25Monday8:00 AM99Student Paper CompetitionBayhill 29/3004K - Department Heads ForumDayTimeSession #Session TitleRoomWednesday8:00 AM453Department Heads Forum (Invited Talks)Bayhill 2204M - Young Faculty ForumDayTimeSession #Session TitleRoom | Monday | 3:30 PM | 217 | NSF Workshop II: Proposal Writing and Discussions with Program Managers | Bayhill 29/30 |
| Sunday 12:30 PM 5 Chem-E-Car Competition Windermere Ballroom Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | 04I - Studen | t Chapters C | Committee Li | aison | |
| Monday 8:00 AM 98 Student Design Competition Bayhill 25 Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Day | Time | Session # | Session Title | Room |
| Monday 8:00 AM 99 Student Paper Competition Bayhill 29/30 O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Sunday | 12:30 PM | 5 | Chem-E-Car Competition | Windermere Ballroom |
| O4K - Department Heads Forum Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 04M - Young Faculty Forum Day Time Session # Session Title Room | Monday | 8:00 AM | 98 | Student Design Competition | Bayhill 25 |
| Day Time Session # Session Title Room Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | Monday | 8:00 AM | 99 | Student Paper Competition | Bayhill 29/30 |
| Wednesday 8:00 AM 453 Department Heads Forum (Invited Talks) Bayhill 22 O4M - Young Faculty Forum Day Time Session # Session Title Room | 04K - Depart | ment Head: | s Forum | | |
| 04M - Young Faculty Forum Day Time Session # Session Title Room | Day | Time | Session # | Session Title | Room |
| Day Time Session # Session Title Room | Wednesday | 8:00 AM | 453 | Department Heads Forum (Invited Talks) | Bayhill 22 |
| | 04M - Young | Faculty For | um | | |
| Wednesday 8:00 AM 493 Young Faculty Forum (Invited Talks) Bayhill 29/30 | Day | Time | Session # | Session Title | Room |
| | Wednesday | 8:00 AM | 493 | Young Faculty Forum (Invited Talks) | Bayhill 29/30 |

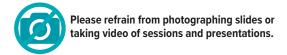


^{*} This session is co-sponsored by one or more programming groups

| Day | Time | Session # | Session Title | Room |
|---------------|--------------|-------------|---|--------------------|
| Monday | 8:00 AM | 83 | Managing in the High Tech World | Bayhill 18 |
| Monday | 12:30 PM | 130 | Digital Twin (Invited Talks)* | Bayhill 28 |
| Tuesday | 8:00 AM | 266 | How We Teach: Ethics, Teamwork, Leadership, and Professional Skills* | Bayhill 23 |
| Tuesday | 8:00 AM | 300 | Woman Chemical Engineers: Managing to Retain Them | Bayhill 18 |
| Tuesday | 12:30 PM | 310 | AIChE Management Award Recipient Presentation Session: Focusing on Technology and Innovation Management | Florida Ballroom C |
| Wednesday | 8:00 AM | 453 | Department Heads Forum (Invited Talks)* | Bayhill 22 |
| Wednesday | 12:30 PM | 508 | Challenges and Best Practices in Technology Commercialization* | Bayhill 18 |
| 05A - Profess | sional Deve | lopment | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 12:30 PM | 130 | Digital Twin (Invited Talks)* | Bayhill 28 |
| Monday | 12:30 PM | 141 | Exploring Ethical Dilemmas in the Workplace: Workshop | Bayhill 18 |
| Monday | 3:30 PM | 212 | How to Prepare Yourself for Management | Bayhill 18 |
| Tuesday | 3:30 PM | 432 | Workshop on Utilizing Leadership Advisory Boards (aka Master Minding) | Bayhill 19 |
| Wednesday | 8:00 AM | 457 | Effective Communication Skills for ChE* | Bayhill 23 |
| 06 - North Ar | nerican Mix | ing Forum | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 87 | Mixing in Rheologically Complex Fluids | Bayhill 32 |
| Monday | 12:30 PM | 153 | Novel and Unconventional Mixers | Bayhill 32 |
| Monday | 3:30 PM | 218 | Numerical Analyses of Mixing Processes in Bioreactors | Bayhill 32 |
| Tuesday | 12:30 PM | 366 | Understanding Mixing Processes I: Advances in CFD and Computational Analysis Tools | Bayhill 32 |
| Tuesday | 3:30 PM | 431 | Understanding Mixing Processes II: Experimental and Computational Investigations | Bayhill 32 |
| Wednesday | 8:00 AM | 470 | Mixing Scale-Up and Scale-Down Issues in Pharmaceutical and Biopharmaceutical Processes | Bayhill 32 |
| Wednesday | 8:00 AM | 491 | Transport Phenomena, Rheology, and Mixing in Food Processing and Engineering (Invited Talks)* | Celebration 9 |
| Wednesday | 12:30 PM | 554 | The Use of CFD in Simulation of Multiphase Mixing Processes | Bayhill 32 |
| Wednesday | 3:30 PM | 597 | North American Mixing Forum Award Session (Invited Talk) | Bayhill 32 |
| 07 - Transpo | rt and Energ | y Processes | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 8 | 3D Printing Applications in Catalysts, Reactions, and Energy Industry* | Bayhill 28 |
| Monday | 3:30 PM | 226 | Redox Flow Batteries for Energy Storage | Bayhill 28 |
| Tuesday | 12:30 PM | 321 | Concentrated Solar Energy for Power Generation and Chemical Processing II* | Regency Ballroom T |
| Tuesday | 12:30 PM | 362 | Thermal Energy Storage | Bayhill 29/30 |
| Tuesday | 3:30 PM | 396 | Concentrated Solar Energy for Power Generation and Chemical Processing III* | Regency Ballroom T |
| Tuesday | 3:30 PM | 404 | Fuel Cells, Electrolyzers, and Electrochemical Devices | Bayhill 29/30 |
| Wednesday | 12:30 PM | 515 | CO ₂ Capture, Utilization, and Disposal: Key to Clean Energy Production | Bayhill 29/30 |
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^{*} This session is co-sponsored by one or more programming groups

| Wednesday | 3:30 PM | 566 | Poster Session: Transport and Energy Processes | Regency Ballroom R/S |
|--------------|--------------|--------------|---|----------------------|
| Thursday | 8:00 AM | 622 | Alternative Fuels including Biofuels, Hydrogen, and Syngas | Bayhill 29/30 |
| Thursday | 12:30 PM | 712 | Transport Processes in Flow Reactors | Bayhill 29/30 |
| Friday | 8:00 AM | 752 | Applied Math for Energy and Environmental Applications* | Celebration 3 |
| 08 - Materia | ls Engineeri | ng and Scien | ces Division | |
| Day | Time | Session # | Session Title | Room |
| Monday | 3:30 PM | 181 | Poster Session: Materials Engineering & Sciences (08A - Polymers) | Regency Ballroom R/S |
| Monday | 3:30 PM | 182 | Poster Session: Materials Engineering & Sciences (08B - Biomaterials) | Regency Ballroom R/S |
| Monday | 3:30 PM | 183 | Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials) | Regency Ballroom R/S |
| Monday | 3:30 PM | 184 | Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials) | Regency Ballroom R/S |
| Monday | 3:30 PM | 185 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials) | Regency Ballroom R/S |
| Monday | 3:30 PM | 215 | Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* | Regency Ballroom Q |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 345 | Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Material Innovations* | Regency Ballroom Q |
| Tuesday | 3:30 PM | 384 | 3D Printing of Composites* | Bayhill 28 |
| Tuesday | 3:30 PM | 429 | Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks)* | Celebration 10 |
| Wednesday | 8:00 AM | 437 | 3D Printing of Functional Materials* | Bayhill 28 |
| Wednesday | 8:00 AM | 455 | Division Plenary: Materials Engineering & Sciences Division (Invited Talks) | Celebration 5 |
| Wednesday | 8:00 AM | 484 | Sensor Development Platforms* | Celebration 10 |
| Wednesday | 12:30 PM | 544 | Practical Applications of Computational Chemistry and Molecular Simulation I* | Rock Spring I/II |
| Wednesday | 3:30 PM | 567 | 3D Printing Fundamental and Applications* | Bayhill 28 |
| Wednesday | 3:30 PM | 603 | Polymers in Additive Manufacturing* | Bayhill 27 |
| Thursday | 12:30 PM | 704 | Practical Applications of Computational Chemistry and Molecular Simulation II* | Rock Spring I/II |
| 08A - Polymo | ers | | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 13 | Atomistic and Molecular Modeling and Simulation of Polymers | Celebration 8 |
| Sunday | 3:30 PM | 20 | Charged Polymers for Membrane-Based Water and Energy Applications* | Barrel Spring II |
| Sunday | 3:30 PM | 34 | Polymers in Industry - Rising Stars (Invited Talks) | Celebration 10 |
| Monday | 8:00 AM | 59 | Charged and Ion-Containing Polymers I | Celebration 11 |
| Monday | 8:00 AM | 89 | Multiscale and Coarse-Grained Modeling of Polymers | Celebration 15 |
| Monday | 12:30 PM | 121 | Charged and Ion-Containing Polymers II | Celebration 11 |
| Monday | 12:30 PM | 157 | Process Innovations on Renewable Polymers and Biobased Intermediates* | Bayhill 17 |
| Monday | 3:30 PM | 181 | Poster Session: Materials Engineering & Sciences (08A - Polymers)* | Regency Ballroom R/S |
| Tuesday | 8:00 AM | 248 | Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering I (Invited Talks) | Celebration 5 |



^{*} This session is co-sponsored by one or more programming groups

| Tuesday | 8:00 AM | 289 | Polymer Networks, Gels, and Crosslinked Systems I | Celebration 11 |
|-------------|----------|-----------|--|----------------------|
| Tuesday | 12:30 PM | 313 | Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering II (Invited Talks) | Celebration 5 |
| Tuesday | 12:30 PM | 355 | Polymers for Energy Storage and Conversion | Celebration 15 |
| Tuesday | 3:30 PM | 384 | 3D Printing of Composites* | Bayhill 28 |
| Tuesday | 3:30 PM | 402 | Excellence in Graduate Polymer Research (Invited Talks) | Celebration 5 |
| Tuesday | 3:30 PM | 415 | Mechanics, Structure, and Properties in Polymers | Celebration 14 |
| Tuesday | 3:30 PM | 420 | Polymer Networks, Gels, and Crosslinked Systems II | Celebration 4 |
| Wednesday | 8:00 AM | 437 | 3D Printing of Functional Materials* | Bayhill 28 |
| Wednesday | 8:00 AM | 484 | Sensor Development Platforms* | Celebration 10 |
| Wednesday | 12:30 PM | 518 | Diffusion in Polymers | Celebration 5 |
| Wednesday | 12:30 PM | 543 | Polymer Thin Films, Nanoconfinement, and Interfaces I | Celebration 11 |
| Wednesday | 3:30 PM | 595 | Nanoscale Structure in Polymers | Celebration 14 |
| Wednesday | 3:30 PM | 602 | Polymer Processing and Rheology | Celebration 5 |
| Wednesday | 3:30 PM | 603 | Polymers in Additive Manufacturing* | Bayhill 27 |
| Wednesday | 3:30 PM | 604 | Polymer Thin Films, Nanoconfinement, and Interfaces II | Celebration 15 |
| Thursday | 8:00 AM | 653 | Polymer Crystallization and Properties of Semi-Crystalline Polymers | Celebration 12/13 |
| Thursday | 8:00 AM | 654 | Polymer Reaction Engineering | Celebration 5 |
| Thursday | 12:30 PM | 673 | Bio-Based Polymers | Celebration 12/13 |
| Thursday | 12:30 PM | 692 | Inhomogeneous Polymers | Celebration 5 |
| Thursday | 3:30 PM | 718 | Biomacromolecular Gels | Celebration 10 |
| Thursday | 3:30 PM | 734 | Nanoscale Phenomena in Macromolecular Systems | Celebration 5 |
| Thursday | 3:30 PM | 747 | Thermodynamics of Polymers | Celebration 12/13 |
| 08B - Bioma | terials | | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 14 | Biomaterials and Life Science Engineering: Faculty Candidates I | Celebration 7 |
| Sunday | 3:30 PM | 15 | Biomimetic Materials I | Celebration 5 |
| Sunday | 3:30 PM | 22 | Engineering in Cancer Biology and Therapy I: Research Tools and Platforms* | Celebration 2 |
| Monday | 8:00 AM | 53 | Biomaterials and Life Science Engineering: Faculty Candidates II | Celebration 7 |
| Monday | 8:00 AM | 55 | Biomimetic Materials II | Celebration 5 |
| Monday | 8:00 AM | 72 | Engineering in Cancer Biology and Therapy II: Mechanisms of Disease* | Celebration 2 |
| Monday | 8:00 AM | 104 | Topical Plenary: Microbial Interactions with Biomaterials and Host Cells (Invited Talks)* | Celebration 9 |
| Monday | 12:30 PM | 114 | Area Plenary: Leaders in Biomaterials (Invited Talks) | Celebration 5 |
| Monday | 12:30 PM | 135 | Emerging Antimicrobial Methods* | Celebration 9 |
| Monday | 12:30 PM | 137 | Engineering in Cancer Biology and Therapy III: Drug Development and Delivery* | Celebration 1 |
| Monday | 12:30 PM | 152 | Nanotechnology and 3D Printing: The Intertwined Technologies* | Discovery 45 |
| Monday | 12:30 PM | 157 | Process Innovations on Renewable Polymers and Biobased Intermediates * | Bayhill 17 |
| Monday | 3:30 PM | 182 | Poster Session: Materials Engineering & Sciences (08B - Biomaterials)* | Regency Ballroom R/S |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research* | Celebration 9 |

^{*} This session is co-sponsored by one or more programming groups

| Tuesday | 0.00 444 | 245 | Applications in Consers Diamodical* | Colobration 10 |
|--------------|--------------|-----------|--|-----------------------------------|
| Tuesday | MA 00:8 | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 8:00 AM | 267 | Hydrogel Biomaterials: Dynamic and Stimuli-Responsive Hydrogels | Celebration 16 |
| Tuesday | 8:00 AM | 282 | Micro- and Nano-Scale Technologies in Life Sciences I* | Celebration 4 |
| Tuesday | 8:00 AM | 293 | Technologies for Understanding Microbial Interactions * | Celebration 9 |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 316 | Biophysical Properties of Microbes and Microbial Communities* | Celebration 9 |
| Tuesday | 12:30 PM | 323 | Data-Driven Design and Modeling of Biomaterials* | Peacock Spring |
| Tuesday | 12:30 PM | 335 | Hydrogel Biomaterials: Cell Culture and Delivery | Celebration 16 |
| Tuesday | 12:30 PM | 346 | Micro- and Nano-Scale Technologies in Life Sciences II* | Celebration 4 |
| Tuesday | 3:30 PM | 384 | 3D Printing of Composites* | Bayhill 28 |
| Tuesday | 3:30 PM | 391 | Biomaterials for Immunological Applications | Celebration 3 |
| Tuesday | 3:30 PM | 392 | Biomaterials: Graduate Student Award Session | Celebration 2 |
| Wednesday | 8:00 AM | 437 | 3D Printing of Functional Materials* | Bayhill 28 |
| Wednesday | 8:00 AM | 447 | Cells, Organs, and Labs on a Chip: Tissue Microenvironments* | Celebration 2 |
| Wednesday | 8:00 AM | 484 | Sensor Development Platforms* | Celebration 10 |
| Wednesday | 12:30 PM | 505 | Biomaterials in Industry and the Clinic | Celebration 16 |
| Wednesday | 12:30 PM | 507 | Cells, Organs, and Labs on a Chip* | Celebration 1 |
| Wednesday | 12:30 PM | 521 | Engineering the Tissue and Cell Microenvironment I: Promoting Functionality and Repair* | Celebration 14 |
| Wednesday | 3:30 PM | 570 | Bioprinting of Scaffolds, Tissues, and Organs | Celebration 12/13 |
| Wednesday | 3:30 PM | 582 | Engineering the Tissue and Cell Microenvironment II: Disease Models and Mechanisms* | Celebration 2 |
| Wednesday | 3:30 PM | 609 | Self-Assembled Biomaterials* | Discovery 44 |
| Thursday | 8:00 AM | 625 | Biomaterial Scaffolds for Tissue Engineering | Celebration 10 |
| Thursday | 8:00 AM | 626 | Biomaterials for Drug Delivery: Controlled Release | Celebration 14 |
| Thursday | 8:00 AM | 628 | Bionanotechnology for Gene and Drug Delivery I* | Discovery 45 |
| Thursday | 8:00 AM | 638 | Drug Delivery I* | Celebration 2 |
| Thursday | 12:30 PM | 674 | Biomaterials | Celebration 10 |
| Thursday | 12:30 PM | 675 | Biomaterials for Drug Delivery: Particles & Colloids | Celebration 14 |
| Thursday | 12:30 PM | 685 | Drug Delivery II* | Celebration 2 |
| Thursday | 3:30 PM | 725 | Drug Delivery III* | Celebration 2 |
| Thursday | 3:30 PM | 735 | Nanostructured Biomimetic and Biohybrid Materials and Devices* | Discovery 45 |
| 08D - Inorga | nic Material | s | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 30 | MOFs, COFs, and Porous Polymer Materials | Celebration 12/13 |
| Monday | 8:00 AM | 101 | Synthesis and Application of Inorganic Materials: Part I | Celebration 16 |
| Monday | 12:30 PM | 167 | Synthesis and Application of Inorganic Materials: Part II | Celebration 16 |
| Monday | 3:30 PM | 183 | Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)* | Regency Ballroom R/ |
| Tuesday | 8:00 AM | 264 | Functional Nanoparticles* | Bayhill 20 |
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 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

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| Wednesday | 8:00 AM | 484 | Sensor Development Platforms* | Celebration 10 |
| Wednesday | 12:30 PM | 528 | Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles* | Bayhill 20 |
| Wednesday | 3:30 PM | 596 | Nanostructured Thin Films | Celebration 16 |
| Thursday | 8:00 AM | 618 | Accelerated Discovery and Development of Inorganic Materials | Celebration 16 |
| Thursday | 12:30 PM | 713 | Two-Dimensional Materials | Celebration 16 |
| 08E - Electro | nics and Ph | otonics | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 45 | Vapor Phase Processing of Materials | Celebration 15 |
| Monday | 12:30 PM | 115 | Area 8E Plenary: Electronic and Photonic Materials: Industry and Academia (Invited Talks) | Celebration 15 |
| Monday | 3:30 PM | 184 | Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)* | Regency Ballroom R/S |
| Tuesday | 8:00 AM | 276 | Materials for Optoelectronic Applications | Celebration 15 |
| Tuesday | 8:00 AM | 293 | Technologies for Understanding Microbial Interactions* | Celebration 9 |
| Tuesday | 3:30 PM | 388 | Area 8E (Electronic and Photonic Materials) Graduate Student Award Session (Sponsored by JVST) | Celebration 15 |
| Wednesday | 8:00 AM | 484 | Sensor Development Platforms* | Celebration 10 |
| Wednesday | 12:30 PM | 556 | Wide Bandgap Materials for Electronic and Photonic Applications | Celebration 15 |
| Thursday | 8:00 AM | 662 | Synthesis and Characterization of Materials for Optical and Electronic Applications | Celebration 15 |
| Thursday | 12:30 PM | 711 | Thermoelectric and Electrochemical Applications of Semiconductors | Celebration 15 |
| 08F - Compo | | | | |
| oor - compo | sites | | | |
| Day | Time | Session # | Session Title | Room |
| | | Session # 185 | Session Title Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* | Room Regency Ballroom R/S |
| Day | Time | | | |
| Day Monday | Time 3:30 PM | 185 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* | Regency Ballroom R/S |
| Day Monday Tuesday | Time 3:30 PM 12:30 PM | 185 317 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites | Regency Ballroom R/S Celebration 11 |
| Day Monday Tuesday Tuesday | Time 3:30 PM 12:30 PM 3:30 PM | 185 317 417 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials | Regency Ballroom R/S Celebration 11 Celebration 11 |
| Day Monday Tuesday Tuesday Wednesday | 3:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM | 185 317 417 484 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and | Regency Ballroom R/S Celebration 11 Celebration 11 Celebration 10 |
| Day Monday Tuesday Tuesday Wednesday Wednesday | Time 3:30 PM 12:30 PM 3:30 PM 8:00 AM 12:30 PM | 185 317 417 484 529 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 |
| Day Monday Tuesday Tuesday Wednesday Wednesday Wednesday | Time 3:30 PM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 3:30 PM | 185 317 417 484 529 574 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 |
| Day Monday Tuesday Tuesday Wednesday Wednesday Wednesday Thursday | Time 3:30 PM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 3:30 PM 8:00 AM 12:30 PM | 185 317 417 484 529 574 649 701 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 |
| Day Monday Tuesday Tuesday Wednesday Wednesday Wednesday Thursday Thursday | Time 3:30 PM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 3:30 PM 8:00 AM 12:30 PM | 185 317 417 484 529 574 649 701 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 |
| Day Monday Tuesday Tuesday Wednesday Wednesday Thursday Thursday Thursday 09 - Environt | 3:30 PM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 8:00 AM 12:30 PM | 185 317 417 484 529 574 649 701 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites Natural and Bio-Composites | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 Celebration 11 Celebration 11 |
| Day Monday Tuesday Tuesday Wednesday Wednesday Thursday Thursday O9 - Environt Day | 3:30 PM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 8:00 AM 12:30 PM Time | 185 317 417 484 529 574 649 701 sion Session # | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites Natural and Bio-Composites Session Title | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Poom Plaza International |
| Day Monday Tuesday Tuesday Wednesday Wednesday Thursday Thursday Thursday O9 - Environt Day Monday | 3:30 PM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 12:30 PM 12:30 PM 8:00 AM | 185 317 417 484 529 574 649 701 Session # | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites Natural and Bio-Composites Session Title Combustion Kinetics and Emissions* Division Plenary: Chemical Engineering Roles in U.S. Department of Energy | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Poom Plaza International Ballroom F |
| Day Monday Tuesday Tuesday Wednesday Wednesday Thursday Thursday Thursday O9 - Environt Day Monday Monday | Time 3:30 PM 12:30 PM 8:00 AM | 185 317 417 484 529 574 649 701 Session # 60 68 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites Natural and Bio-Composites Session Title Combustion Kinetics and Emissions* Division Plenary: Chemical Engineering Roles in U.S. Department of Energy Environmental Management and Waste Cleanup Programs* | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Celebration 15 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Celebration 11 |
| Day Monday Tuesday Tuesday Wednesday Wednesday Thursday Thursday O9 - Environ Day Monday Monday Monday | Time 3:30 PM 12:30 PM 8:00 AM 12:30 PM 8:00 AM 12:30 PM 8:00 AM 12:30 PM mental Divis Time 8:00 AM 8:00 AM 12:30 PM | 185 317 417 484 529 574 649 701 sion Session # 60 68 139 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites Natural and Bio-Composites Session Title Combustion Kinetics and Emissions* Division Plenary: Chemical Engineering Roles in U.S. Department of Energy Environmental Management and Waste Cleanup Programs* Environmental Division Awards and Honors (Invited Talks) | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Celebration 17 Celebration 11 Celebration 11 Room Plaza International Ballroom F Challenger 41/42 Blue Spring I/II |
| Day Monday Tuesday Tuesday Wednesday Wednesday Thursday Thursday Thursday O9 - Environt Day Monday Monday Monday Monday | Time 3:30 PM 12:30 PM 8:00 AM 12:30 PM | 185 317 417 484 529 574 649 701 Session # 60 68 139 166 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* Characterization of Composites Nanocomposites with 2D Materials Sensor Development Platforms* Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion* Composites for Energy and Environmental Applications Multifunctional Composites Natural and Bio-Composites Session Title Combustion Kinetics and Emissions* Division Plenary: Chemical Engineering Roles in U.S. Department of Energy Environmental Management and Waste Cleanup Programs* Environmental Division Awards and Honors (Invited Talks) Sustainable Management and Uses of Post-Consumer Materials and Waste* | Regency Ballroom R/S Celebration 11 Celebration 10 Discovery 44 Celebration 11 Celebration 11 Celebration 11 Celebration 11 Celebration 15 Celebration 11 Room Plaza International Ballroom F Challenger 41/42 Blue Spring I/II Regency Ballroom U |

^{*} This session is co-sponsored by one or more programming groups

| Wednesday | 8:00 AM | 461 | Heterogeneous Catalysis in Liquid Media I* | Florida Ballroom A |
|---------------|------------|-----------|--|-----------------------------------|
| Wednesday | 3:30 PM | 562 | Poster Session: Environmental Division | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 587 | Integrated Process Engineering and Economic Analysis* | Regency Ballroom Q |
| Friday | 8:00 AM | 752 | Applied Math for Energy and Environmental Applications* | Celebration 3 |
| 09A - Air | | | | |
| Day | Time | Session # | Session Title | Room |
| Wednesday | 8:00 AM | 445 | Atmospheric Chemistry and Physics: Laboratory Studies | Blue Spring I/II |
| Wednesday | 12:30 PM | 503 | Atmospheric Chemistry and Physics: Modeling and Field Studies | Blue Spring I/II |
| 09B - Water | | | | |
| Day | Time | Session # | Session Title | Room |
| Wednesday | 12:30 PM | 512 | Community-Based Water Treatment Innovations | Rainbow Spring I/II |
| Thursday | 8:00 AM | 620 | Advanced Treatment for Water: Reuse and Recycling | Rainbow Spring I/II |
| Thursday | 8:00 AM | 665 | Water Treatment, Desalination, and Reuse I* | Barrel Spring I |
| Thursday | 12:30 PM | 670 | Advanced Treatment for Water: Advanced Oxidation Processes | Rainbow Spring I/II |
| 09C - Solid a | nd Hazardo | us Waste | | |
| Day | Time | Session # | Session Title | Room |
| Tuesday | 12:30 PM | 309 | Advances in Nuclear and Hazardous Waste Processing and Disposal* | Discovery 43 |
| Tuesday | 12:30 PM | 332 | Fundamentals and Applications for Hazardous Waste Treatment | Blue Spring I/II |
| Tuesday | 3:30 PM | 397 | Conversion of Solid Wastes to Energy and/or Product* | Regency Ballroom Q |
| Tuesday | 3:30 PM | 405 | Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization | Blue Spring I/II |
| 09D - Proces | s Developm | ent | | |
| Day | Time | Session # | Session Title | Room |
| Tuesday | 8:00 AM | 241 | Advances in Life Cycle Optimization for Process Development | Blue Spring I/II |
| 09F - Fundar | mentals | | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 24 | Fundamentals of Food, Energy, and Water Systems | Blue Spring I/II |
| Monday | 8:00 AM | 76 | Fundamentals of Environmental Kinetics and Reaction Engineering | Blue Spring I/II |
| Monday | 3:30 PM | 209 | Fundamentals of Sustainability Science and Engineering | Blue Spring I/II |
| 09G - Sustaiı | nability | | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering* | Regency Ballroom O |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G |
| Wednesday | 8:00 AM | 459 | Environmentally Friendly Product and Process Development for Sustainability* | Bayhill 18 |
| Wednesday | 8:00 AM | 488 | Sustainable Fuel from Renewable Resources | Rainbow Spring I/II |
| Thursday | 8:00 AM | 634 | CO ₂ Industrial, Engineering and R&D Approaches | Blue Spring I/II |
| Thursday | 8:00 AM | 661 | Sustainability and Consumer Products* | Regency Ballroom V |
| Thursday | 12:30 PM | 691 | Going to a Decision Point in Sustainability Analysis | Blue Spring I/II |
| | | | | |

 $[\]ensuremath{^{*}}$ This session is co-sponsored by one or more programming groups

| 09H - Climat | e Change | | | |
|--------------|-------------|-------------|--|---------------------|
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 57 | Carbon Dioxide Capture Technologies and Their Use | Rainbow Spring I/II |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering* | Regency Ballroom O |
| 10 - Computi | ng Systems | and Technol | logy Division | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 41 | Software Tools and Implementations for Process Systems Engineering | Bayhill 26 |
| Monday | 8:00 AM | 51 | Big Data and Analytics for Sustainability* | Regency Ballroom T |
| Monday | 8:00 AM | 52 | Big Data and Data Analytics (Invited Talks)* | Bayhill 27 |
| Monday | 8:00 AM | 66 | Division Plenary: CAST (Invited Talks) | Regency Ballroom O |
| Monday | 8:00 AM | 80 | Industrial Applications of Integrated Synthesis, Design and Operations Through Modeling and Optimization* | Bayhill 17 |
| Monday | 12:30 PM | 118 | CAST Director's Student Presentation Award Finalists (Invited Talks) | Bayhill 24 |
| Monday | 12:30 PM | 128 | Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II* | Regency Ballroom V |
| Monday | 12:30 PM | 145 | Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond* | Bayhill 27 |
| Monday | 3:30 PM | 195 | Applications of Data Science in Molecular Sciences I* | Peacock Spring |
| Monday | 3:30 PM | 200 | Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III* | Regency Ballroom V |
| Tuesday | 8:00 AM | 263 | Computing for ChEs: Teaching Programming and Simulation Software* | Bayhill 29/30 |
| Tuesday | 8:00 AM | 269 | Industry 4.0 and Digital Transformation (Invited Talks)* | Bayhill 27 |
| Tuesday | 8:00 AM | 273 | In Honor of the 2018 Recipient of the Warren K. Lewis Award (Invited Talks)* | Bayhill 22 |
| Tuesday | 3:30 PM | 389 | Artificial Intelligence and Advanced Computation* | Bayhill 27 |
| Tuesday | 3:30 PM | 411 | Innovations in Methods of Data Science* | Peacock Spring |
| Wednesday | 12:30 PM | 502 | Applications of Data Science in Molecular Sciences II* | Peacock Spring |
| Wednesday | 12:30 PM | 516 | Data Science Education in Chemical Engineering Panel Discussion* | Manatee Spring I |
| Wednesday | 12:30 PM | 544 | Practical Applications of Computational Chemistry and Molecular Simulation I* | Rock Spring I/II |
| Wednesday | 3:30 PM | 571 | CACHE 50th Anniversary: The Future of Cyber-Assisted Chemical Engineering Education* | Regency Ballroom T |
| Wednesday | 3:30 PM | 587 | Integrated Process Engineering and Economic Analysis* | Regency Ballroom G |
| Thursday | 8:00 AM | 657 | PSE Methods for Safety and Reliability | Bayhill 26 |
| Thursday | 12:30 PM | 704 | Practical Applications of Computational Chemistry and Molecular Simulation II* | Rock Spring I/II |
| 10A - System | s and Proce | ess Design | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 62 | Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I* | Regency Ballroom V |
| Monday | 8:00 AM | 80 | Industrial Applications of Integrated Synthesis, Design and Operations Through Modeling and Optimization* | Bayhill 17 |
| Monday | 12:30 PM | 112 | Advances in Process Design I | Bayhill 25 |
| Monday | 12:30 PM | 145 | Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond* | Bayhill 27 |
| Tuesday | 8:00 AM | 263 | Computing for ChEs: Teaching Programming and Simulation Software* | Bayhill 29/30 |
| Tuesday | 8:00 AM | 271 | In Honor of Professor Ignacio Grossmann's 70th Birthday - I (Invited Talks) | Bayhill 24 |
| Tuesday | 8:00 AM | 294 | The Energy-Water Nexus* | Regency Ballroom V |

^{*} This session is co-sponsored by one or more programming groups

| Tuesday | 12:30 PM | 325 | Design for a Circular Economy* | Regency Ballroom U |
|--------------|---------------|---------------|--|----------------------|
| Tuesday | 12:30 PM | 361 | The Food-Energy-Water Nexus* | Regency Ballroom V |
| Tuesday | 3:30 PM | 372 | Interactive Session: Systems and Process Design | Regency Ballroom R/S |
| Wednesday | 8:00 AM | 463 | In Honor of Professor Rafiqui Gani's 65th Birthday (Invited Talks) | Bayhill 24 |
| Wednesday | 12:30 PM | 500 | Advances in Process Design II | Bayhill 24 |
| Wednesday | 3:30 PM | 576 | Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems* | Challenger 41/42 |
| Wednesday | 3:30 PM | 606 | Process Intensification through Process Systems Engineering | Bayhill 24 |
| Thursday | 8:00 AM | 635 | Design and Operations Under Uncertainty | Bayhill 25 |
| Thursday | 12:30 PM | 706 | Process Design: Innovation for Sustainability* | Regency Ballroom V |
| Thursday | 3:30 PM | 739 | Process Design in Energy and Sustainability | Bayhill 26 |
| Friday | 12:30 PM | 763 | Integrated Product and Process Design | Celebration 2 |
| 10B - System | s and Proce | ess Control | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 29 | Modeling, Control, and Optimization of Manufacturing Systems | Bayhill 25 |
| Monday | 12:30 PM | 145 | Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond* | Bayhill 27 |
| Monday | 3:30 PM | 199 | Data-Driven Techniques for Dynamic Modeling, Estimation, and Control I | Bayhill 25 |
| Tuesday | 8:00 AM | 243 | Advances in Process Control | Bayhill 25 |
| Tuesday | 8:00 AM | 263 | Computing for ChEs: Teaching Programming and Simulation Software* | Bayhill 29/30 |
| Tuesday | 8:00 AM | 284 | Modeling and Control of Crystallization I* | Coral Spring I/II |
| Tuesday | 12:30 PM | 324 | Data-Driven Techniques for Dynamic Modeling, Estimation, and Control II | Bayhill 25 |
| Tuesday | 3:30 PM | 371 | Interactive Session: Systems and Process Control | Regency Ballroom R/S |
| Wednesday | 8:00 AM | 452 | Cybersecurity* | Bayhill 27 |
| Wednesday | 12:30 PM | 504 | Big Data and Applications in Advanced Modeling and Manufacturing* | Bayhill 27 |
| Wednesday | 12:30 PM | 522 | Estimation and Control Under Uncertainty | Bayhill 25 |
| Wednesday | 3:30 PM | 591 | Modeling, Control, and Optimization of Energy Systems | Bayhill 25 |
| Thursday | 12:30 PM | 705 | Predictive Control and Optimization | Bayhill 25 |
| Thursday | 3:30 PM | 740 | Process Modeling and Control Applications I | Bayhill 25 |
| Friday | 12:30 PM | 767 | Process Modeling and Control Applications II | Celebration 3 |
| 10C - Compu | iters in Opei | rations and I | nformation Processing | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 26 | Industrial Applications in Design and Operations | Bayhill 24 |
| Monday | 3:30 PM | 194 | Advances in Optimization: Global, Uncertainty, Surrogate & Mixed-Integer Models I | Bayhill 24 |
| Tuesday | 8:00 AM | 263 | Computing for ChEs: Teaching Programming and Simulation Software* | Bayhill 29/30 |
| Tuesday | 12:30 PM | 339 | In Honor of Professor Ignacio Grossmann's 70th Birthday - II (Invited Talks) | Bayhill 24 |
| Tuesday | 3:30 PM | 373 | Interactive Session: Systems and Process Operations | Regency Ballroom R/S |
| Wednesday | 8:00 AM | 442 | Advances in Supply Chain Design and Logistics | Bayhill 25 |



An up-to-date program is available at aiche.org/annual or on the AIChEvents app.

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| Wednesday | 3:30 PM | 575 | Data Driven Optimization | Bayhill 26 |
|---------------|--------------|------------|---|----------------------|
| Thursday | 8:00 AM | 621 | Advances in Optimization: Global, Surrogate & Mixed-Integer Models II | Bayhill 24 |
| Thursday | 12:30 PM | 708 | Supply Chain Management and Scheduling | Bayhill 24 |
| Thursday | 3:30 PM | 737 | Operation of Energy Systems | Bayhill 24 |
| Friday | 8:00 AM | 751 | Advances in Optimization and Planning | Celebration 2 |
| Friday | 12:30 PM | 769 | Real-Time Optimization of Operations | Celebration 1 |
| , | | | erical Analysis | Gelebration 1 |
| Day | Time | Session # | Session Title | Room |
| Monday | 12:30 PM | 110 | Advances in Computational Methods and Numerical Analysis | Bayhill 26 |
| Tuesday | 8:00 AM | 263 | Computing for ChEs: Teaching Programming and Simulation Software* | Bayhill 29/30 |
| Tuesday | 8:00 AM | 272 | In Honor of Prof. Yannis G. Kevrekidis' 60th Birthday (Invited Talks) | Bayhill 26 |
| Tuesday | 3:30 PM | 369 | Interactive Session: Applied Mathematics and Numerical Analysis | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 389 | Artificial Intelligence and Advanced Computation* | Bayhill 27 |
| Wednesday | 8:00 AM | 444 | Applied Math for Biological and Biomedical Systems | Bayhill 26 |
| Friday | 8:00 AM | 752 | Applied Math for Energy and Environmental Applications | Celebration 3 |
| 10E - Data ar | nd Informati | on Systems | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 11 | Advanced Modelling and Data Systems Applications in Next-Gen Manufacturing* | Bayhill 27 |
| Monday | 8:00 AM | 51 | Big Data and Analytics for Sustainability* | Regency Ballroom T |
| Monday | 8:00 AM | 52 | Big Data and Data Analytics (Invited Talks)* | Bayhill 27 |
| Monday | 12:30 PM | 145 | Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond* | Bayhill 27 |
| Monday | 3:30 PM | 193 | Advances in Machine Learning Methods for Process Systems Engineering | Bayhill 26 |
| Monday | 3:30 PM | 195 | Applications of Data Science in Molecular Sciences I* | Peacock Spring |
| Tuesday | 8:00 AM | 246 | Applications of Data Science in Catalysis and Reaction Engineering I* | Peacock Spring |
| Tuesday | 8:00 AM | 259 | Data Science & Analytics for Operations Support and Predictions in Pharmaceutical Processes & Products* | Celebration 6 |
| Tuesday | 12:30 PM | 323 | Data-Driven Design and Modeling of Biomaterials* | Peacock Spring |
| Tuesday | 12:30 PM | 344 | Machine Learning Applications and Intelligent Systems | Bayhill 26 |
| Tuesday | 3:30 PM | 370 | Interactive Session: Data and Information Systems | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 389 | Artificial Intelligence and Advanced Computation* | Bayhill 27 |
| Tuesday | 3:30 PM | 411 | Innovations in Methods of Data Science* | Peacock Spring |
| Tuesday | 3:30 PM | 423 | Process-wide and Operational Topics* | Celebration 6 |
| Wednesday | 8:00 AM | 443 | Applications of Data Science in Catalysis and Reaction Engineering II* | Peacock Spring |
| Wednesday | 12:30 PM | 502 | Applications of Data Science in Molecular Sciences II* | Peacock Spring |
| Wednesday | 12:30 PM | 504 | Big Data and Applications in Advanced Modeling and Manufacturing* | Bayhill 27 |
| Wednesday | 12:30 PM | 546 | Process Monitoring & Fault Detection | Bayhill 26 |
| Thursday | 12:30 PM | 672 | Big-Data for Process Applications | Bayhill 26 |
| Friday | 8:00 AM | 753 | Data-Driven and Hybrid Modeling for Decision Making | Celebration 1 |

^{*} This session is co-sponsored by one or more programming groups

| Day | Time | Session # | Session Title | Room |
|----------------|--------------|--------------|---|-----------------------------------|
| Monday | 12:30 PM | 168 | The Path Less Traveled: Professional Development for Non-Tenure Track Faculty* | Bayhill 22 |
| Tuesday | 8:00 AM | 269 | Industry 4.0 and Digital Transformation (Invited Talks)* | Bayhill 27 |
| Wednesday | 11:15 AM | 495 | John M. Prausnitz AIChE Institute Lecture* | Plaza International Ballroom H |
| Wednesday | 3:30 PM | 564 | Poster Session: Process Development | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 587 | Integrated Process Engineering and Economic Analysis* | Regency Ballroom Q |
| Thursday | 8:00 AM | 642 | In-Silico Tools for Accelerating Pharmaceutical Process Development* | Celebration 7 |
| 12A - Proces | s Research | and Innovati | on | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 80 | Industrial Applications of Integrated Synthesis, Design and Operations Through Modeling and Optimization | Bayhill 17 |
| Monday | 12:30 PM | 130 | Digital Twin (Invited Talks)* | Bayhill 28 |
| Monday | 12:30 PM | 157 | Process Innovations on Renewable Polymers and Biobased Intermediates | Bayhill 17 |
| Tuesday | 8:00 AM | 258 | Conceptual Process Design in Refining, Petrochemicals and Gas Processing* | Challenger 38/39 |
| Tuesday | 8:00 AM | 287 | PAT and Process Monitoring in Crystallization Development and Manufacturing* | Manatee Spring I |
| Tuesday | 12:30 PM | 366 | Understanding Mixing Processes I: Advances in CFD and Computational Analysis Tools* | Bayhill 32 |
| Tuesday | 3:30 PM | 410 | Innovations and Emerging Technologies: Drug Substance and Drug Product Development* | Celebration 8 |
| Tuesday | 3:30 PM | 422 | Process Research for Improved Throughput & Efficiency, and Reduced Cost | Bayhill 18 |
| Wednesday | 8:00 AM | 459 | Environmentally Friendly Product and Process Development for Sustainability | Bayhill 18 |
| Wednesday | 3:30 PM | 567 | 3D Printing Fundamental and Applications* | Bayhill 28 |
| 12B - Pilot Pl | ants | | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 12:30 PM | 130 | Digital Twin (Invited Talks)* | Bayhill 28 |
| Wednesday | 8:00 AM | 470 | Mixing Scale-Up and Scale-Down Issues in Pharmaceutical and Biopharmaceutical Processes* | Bayhill 32 |
| 12C - Techno | logy Transfe | er and Manu | facturing | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 29 | Modeling, Control, and Optimization of Manufacturing Systems* | Bayhill 25 |
| Monday | 12:30 PM | 130 | Digital Twin (Invited Talks)* | Bayhill 28 |
| Monday | 12:30 PM | 145 | Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond* | Bayhill 27 |
| Tuesday | 3:30 PM | 389 | Artificial Intelligence and Advanced Computation* | Bayhill 27 |
| Wednesday | 12:30 PM | 508 | Challenges and Best Practices in Technology Commercialization | Bayhill 18 |
| Thursday | 8:00 AM | 645 | Manufacturing Process Improvements for Chemical/Petrochemical Industries | Bayhill 18 |
| Thursday | 12:30 PM | 677 | Case Studies in Technology: Design, Risk Reduction and Implementation | Bayhill 18 |



 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| Day | Time | Session # | Session Title | Room |
|---------------|-------------|--------------|---|--------------------|
| Wednesday | 8:00 AM | 441 | Advances in Process Intensification | Bayhill 17 |
| Wednesday | 12:30 PM | 545 | Process Intensification By Enhanced Heat and Mass Transfer | Bayhill 17 |
| Thursday | 8:00 AM | 656 | Process Intensification By Process Integration | Bayhill 17 |
| Thursday | 12:30 PM | 707 | Process Intensification through the Application of Microreactors, Multiphase Reactors, and Membrane Reactors | Bayhill 17 |
| 12G - Produc | t Design | | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 33 | Panel Discussion: Chemical Process and Product Design Careers in Industry & Academia (Invited Talks) | Bayhill 17 |
| Monday | 3:30 PM | 229 | Sustainable and Green Product Design | Bayhill 17 |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 8:00 AM | 260 | Development of Pharmaceutical Process Control Strategies for Drug Product Manufacture* | Celebration 8 |
| Tuesday | 8:00 AM | 295 | Tools and Techniques for Product Design | Bayhill 17 |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 329 | Experiences in Teaching Process Safety I | Bayhill 17 |
| Tuesday | 3:30 PM | 403 | Experiences in Teaching Process Safety II | Bayhill 17 |
| Wednesday | 8:00 AM | 484 | Sensor Development Platforms* | Celebration 10 |
| Wednesday | 3:30 PM | 577 | Development of Pharmaceutical Process Control Strategies for Drug Substance Manufacture* | Celebration 8 |
| Thursday | 12:30 PM | 683 | Development of Pharmaceutical Process Control Strategies for Production of Biologics* | Celebration 6 |
| 14 - Nuclear | Engineering | Division | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 68 | Division Plenary: Chemical Engineering Roles in U.S. Department of Energy Environmental Management and Waste Cleanup Programs | Challenger 41/42 |
| Monday | 3:30 PM | 172 | Wilson Award Winner (Invited Talks) | Discovery 43 |
| Monday | 4:15 PM | 233 | Tutorial on Nuclear Chemical Engineering Focusing on Nuclear Fuel Cycle (Invited Talks) | Discovery 43 |
| Tuesday | 8:00 AM | 242 | Advances in Nuclear Separation Processes and Applications | Discovery 43 |
| Tuesday | 12:30 PM | 309 | Advances in Nuclear and Hazardous Waste Processing and Disposal | Discovery 43 |
| Tuesday | 3:30 PM | 385 | Advanced Nuclear Energy Applications for Molten Salts | Discovery 43 |
| Wednesday | 8:00 AM | 489 | Theory, Modeling, and Simulation of Nuclear Chemical Processes I | Discovery 43 |
| Wednesday | 12:30 PM | 551 | Theory, Modeling, and Simulation of Nuclear Chemical Processes II | Discovery 43 |
| 15 - Food, Ph | narmaceutic | al & Bioengi | neering Division | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 12 | Advances in Enzymatic Catalysis* | Florida Ballroom A |
| Sunday | 3:30 PM | 14 | Biomaterials and Life Science Engineering: Faculty Candidates I* | Celebration 7 |
| Sunday | 3:30 PM | 42 | Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond* | Coral Spring I/II |

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| Monday | 8:00 AM | 74 | Forum Plenary: Opportunities and Challenges with Journey from Industry 4.0 to Pharma 4.0* | Celebration 6 |
|-----------|----------|-----|---|----------------------|
| Monday | 8:00 AM | 104 | Topical Plenary: Microbial Interactions with Biomaterials and Host Cells (Invited Talks)* | Celebration 9 |
| Monday | 12:30 PM | 124 | Computational Solid State Pharmaceutics* | Celebration 7 |
| Monday | 12:30 PM | 126 | Continuous Processing in Drug Substance* | Celebration 6 |
| Monday | 3:30 PM | 189 | Poster Session: Pharmaceutical* | Regency Ballroom R/S |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research* | Celebration 9 |
| Monday | 6:30 PM | 237 | Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony* | Regency Ballroom U |
| Tuesday | 8:00 AM | 240 | Advances in Large Molecule Processes* | Celebration 7 |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 8:00 AM | 259 | Data Science & Analytics for Operations Support and Predictions in Pharmaceutical Processes & Products* | Celebration 6 |
| Tuesday | 8:00 AM | 260 | Development of Pharmaceutical Process Control Strategies for Drug Product Manufacture* | Celebration 8 |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 322 | Continuous Drug Substance Isolation* | Celebration 6 |
| Tuesday | 12:30 PM | 340 | Innovations in Particle Engineering: From Amorphous Solid Dispersions to New Processing* | Celebration 7 |
| Tuesday | 12:30 PM | 342 | Integrated Design for Drug Substance Synthesis* | Celebration 8 |
| Tuesday | 12:30 PM | 354 | Pharma 4.0 (Invited Talks)* | Bayhill 27 |
| Tuesday | 3:30 PM | 399 | Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks) | Regency Ballroom V |
| Tuesday | 3:30 PM | 410 | Innovations and Emerging Technologies: Drug Substance and Drug Product Development* | Celebration 8 |
| Tuesday | 3:30 PM | 421 | Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals I* | Celebration 7 |
| Tuesday | 3:30 PM | 423 | Process-wide and Operational Topics* | Celebration 6 |
| Tuesday | 3:30 PM | 429 | Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks)* | Celebration 10 |
| Wednesday | 8:00 AM | 444 | Applied Math for Biological and Biomedical Systems* | Bayhill 26 |
| Wednesday | 8:00 AM | 451 | Continuous Processing Technologies Applied in Drug Product Manufacturing* | Celebration 7 |
| Wednesday | 8:00 AM | 471 | Modeling and Design of Biopharmaceutical Processes* | Celebration 8 |
| Wednesday | 8:00 AM | 478 | Panel on Pre-Competitive Collaboration (Invited Talks)* | Celebration 6 |
| Wednesday | 8:00 AM | 492 | Understanding Powder Processing via Materials Science* | Celebration 14 |
| Wednesday | 12:30 PM | 496 | 3D Printing in Pharmaceutical and Health Industry* | Bayhill 28 |
| Wednesday | 12:30 PM | 499 | Advances in Drug Discovery Processes* | Celebration 7 |
| Wednesday | 12:30 PM | 509 | Characterization of Continuous Drug Product Unit Operations* | Celebration 6 |
| Wednesday | 12:30 PM | 533 | Integrated Design for Solid Drug Products* | Celebration 8 |

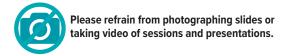


^{*} This session is co-sponsored by one or more programming groups

| Monday | 12:30 PM | 109 | Advances in Biosensors and Biodiagnostics: Biosensor and Biodiagnostic Detection Methods | Celebration 4 |
|--------------|--------------------|-----------|---|-------------------------------------|
| Monday | O.UU AIVI | 104 | (Invited Talks)* | Celebianoli 3 |
| | 8:00 AM | 104 | Topical Plenary: Microbial Interactions with Biomaterials and Host Cells | Celebration 9 |
| Monday | 8:00 AM | 102 | Synthetic Biology: Design Principles and Tool Development in Gene Regulation | Celebration 3 |
| Monday | 8:00 AM | 94 | Regenerative Engineering: Substrate-Derived Control of Cellular Behavior* | Celebration 8 |
| Monday | 8:00 AM | 86 | Metabolic Engineering of Non-Model Organisms | Celebration 4 |
| Monday | 8:00 AM | 79 | Gene Regulation Engineering: Applications in Medicine and Biotechnology | Celebration 14 |
| Monday | 8:00 AM | 70 | Efficient Biological Processing of Lignin to Bioproducts and Biofuels* | Regency Ballroom Q |
| Sunday | 3:30 PM 3:30 PM | 32 | Conversion for Bulk Chemicals New Tools and Applications from Unconventional Synthetic Biology Organisms | Celebration 4 Celebration 14 |
| Day | | | Metabolic Engineering: Biosynthetic Pathway Engineering and Enzymatic | |
| 15C - Bioeng | Time | Session # | Session Title | Room |
| | | | piopriantiaceutical Processes. | |
| Wednesday | 8:00 AM | 470 | Mixing Scale-Up and Scale-Down Issues in Pharmaceutical and Biopharmaceutical Processes* | Bayhill 32 |
| Tuesday | 3:30 PM | 399 | Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)* | Regency Ballroom V |
| Monday | 3:30 PM | 198 | Crystallization of Pharmaceutical and Biological Molecules* | Coral Spring I/II |
| Monday | 8:00 AM | 69 | Division Plenary: Gerhold and Kunesh Awards on Separations (Invited Talks)* | Manatee Spring II |
| Sunday | 3:30 PM | 42 | Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond* | Coral Spring I/II |
| Sunday | 3:30 PM | 12 | Advances in Enzymatic Catalysis* | Florida Ballroom A |
| Day | Time | Session # | Session Title | Room |
| 15B - Pharma | | 000 | 1100000 Engineering in 1 ood and proprocess industries | - Colebiation i |
| Thursday | 8:00 AM | 655 | Process Engineering in Food and Bioprocess Industries | Celebration 1 |
| Tuesday | 12:30 PM | 347 | Microbiomes and Metabolomes in Food, Health, and Bioprocessing | Celebration 1 |
| Tuesday | 8:00 AM | 279 | Membrane Technology in Food and Bioprocess Engineering | Celebration 1 |
| Monday | 3:30 PM | 178 | Poster Session: Food and bioprocess Engineering Poster Session: Food Innovation and Engineering* | Regency Ballroom R/S |
| Monday | 8:00 AM 3:30 PM | 177 | Poster Session: Food and Bioprocess Engineering | Celebration 1 Regency Ballroom R/S |
| Sunday | 3:30 PM | 17 85 | Biotechnological Production of Food and Feed Ingredients Metabolic Engineering for Food, Feed, and Bioproducts | Celebration 1 |
| Day | Time | Session # | Session Title | Room |
| 15A - Food | Time | Carai " | Consider Title | D |
| Thursday | 12:30 PM | 693 | Innovations and Emerging Technologies: Automated Platforms and Novel Methodologies* | Celebration 7 |
| Thursday | 12:30 PM | 683 | Development of Pharmaceutical Process Control Strategies for Production of Biologics* | Celebration 6 |
| Thursday | 8:00 AM | 642 | In-Silico Tools for Accelerating Pharmaceutical Process Development* | Celebration 7 |
| Thursday | 8:00 AM | 640 | Enabling and Advancing Formulations in Drug Product* | Celebration 6 |
| Wednesday | 3:30 PM | 605 | Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals II* | Celebration 7 |
| Wednesday | 3:30 PM | 600 | Particle Engineering and Crystallization in Materials Science* | Celebration 6 |
| Wednesday | 3:30 PM | 577 | Development of Pharmaceutical Process Control Strategies for Drug Substance Manufacture* | Celebration 8 |

^{*} This session is co-sponsored by one or more programming groups

| Monday | 12:30 PM | 134 | Efficient Chemical Processing of Lignin to Bioproducts and Biofuels* | Regency Ballroom Q |
|-----------|----------|-----|---|-----------------------------------|
| Monday | 12:30 PM | 135 | Emerging Antimicrobial Methods* | Celebration 9 |
| Monday | 12:30 PM | 149 | Metabolic Engineering of Autotrophs | Celebration 2 |
| Monday | 12:30 PM | 160 | Regenerative Engineering: Stem Cells and Mechanotransduction* | Celebration 8 |
| Monday | 3:30 PM | 175 | Poster Session: Bioengineering | Regency Ballroom R/S |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research* | Celebration 9 |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 8:00 AM | 280 | Metabolic Engineering: Biosynthetic Pathway Engineering and Enzymatic Conversion for Fine Chemicals | Celebration 3 |
| Tuesday | 8:00 AM | 281 | Metabolic Engineering: Emerging Tools and Technologies | Celebration 2 |
| Tuesday | 8:00 AM | 285 | Multiscale Systems Biology* | Celebration 14 |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G |
| Tuesday | 12:30 PM | 306 | Advances in Biosensors and Biodiagnostics: Systems and Devices for Advanced Biosensing | Celebration 3 |
| Tuesday | 12:30 PM | 307 | Advances in Cell Culture Engineering and Biopharmaceutical Manufacturing | Celebration 14 |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 316 | Biophysical Properties of Microbes and Microbial Communities* | Celebration 9 |
| Wednesday | 8:00 AM | 438 | Advances in Biosynthesis: Chemi-Enzymatic Conversion | Celebration 4 |
| Wednesday | 8:00 AM | 466 | Mammalian Synthetic Biology | Celebration 3 |
| Wednesday | 12:30 PM | 498 | Advances in Bioprocess Design for Cell Culture and Bioproduct Production | Celebration 4 |
| Wednesday | 12:30 PM | 548 | Protein Science and Engineering: Advances on Engineering the Physiochemical Properties of Proteins | Celebration 3 |
| Wednesday | 12:30 PM | 549 | Systems and Quantitative Biology: Signaling Pathways, Response Networks and Growth | Celebration 2 |
| Wednesday | 3:30 PM | 605 | Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals II* | Celebration 7 |
| Wednesday | 3:30 PM | 607 | Protein Engineering* | Celebration 1 |
| Wednesday | 3:30 PM | 608 | Protein Science and Engineering: High Throughput Screening and Characterization | Celebration 3 |
| Wednesday | 3:30 PM | 612 | Systems and Quantitative Biology: Modeling Biological Processes | Celebration 4 |
| Thursday | 8:00 AM | 627 | Biomedical Applications of Protein Engineering | Celebration 3 |
| Thursday | 8:00 AM | 663 | Systems and Quantitative Biology: From Communities to Single Cells | Celebration 4 |
| Thursday | 12:30 PM | 671 | Advances in Biocatalysis : Bioprospecting and Enzyme Engineering | Celebration 1 |
| Thursday | 12:30 PM | 681 | Computational Approaches to Protein Engineering | Celebration 3 |
| Thursday | 12:30 PM | 710 | Systems and Quantitative Biology: Drugs and Small Molecules | Celebration 4 |
| Thursday | 3:30 PM | 719 | Biomolecular Engineering* | Celebration 3 |
| Thursday | 3:30 PM | 736 | Omics and High-Throughput Technologies* | Celebration 1 |

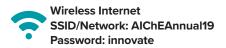


^{*} This session is co-sponsored by one or more programming groups

| 15D - Engine | ering Funda | mentals in L | ife Science | |
|--------------|-------------|--------------|--|----------------------|
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 19 | Cell Biomechanics and Adhesion | Celebration 3 |
| Sunday | 3:30 PM | 22 | Engineering in Cancer Biology and Therapy I: Research Tools and Platforms | Celebration 2 |
| Monday | 8:00 AM | 72 | Engineering in Cancer Biology and Therapy II: Mechanisms of Disease | Celebration 2 |
| Monday | 8:00 AM | 79 | Gene Regulation Engineering: Applications in Medicine and Biotechnology* | Celebration 14 |
| Monday | 12:30 PM | 137 | Engineering in Cancer Biology and Therapy III: Drug Development and Delivery | Celebration 1 |
| Monday | 12:30 PM | 138 | Engineering in Development and Aging | Celebration 3 |
| Monday | 12:30 PM | 158 | Quantitative Approaches to Disease Mechanisms and Therapies | Celebration 14 |
| Monday | 3:30 PM | 176 | Poster Session: Engineering Fundamentals in Life Science | Regency Ballroom R/S |
| Tuesday | 8:00 AM | 282 | Micro- and Nano-Scale Technologies in Life Sciences I | Celebration 4 |
| Tuesday | 8:00 AM | 285 | Multiscale Systems Biology | Celebration 14 |
| Tuesday | 12:30 PM | 311 | Applications in Immunology and Immunotherapy | Celebration 2 |
| Tuesday | 12:30 PM | 346 | Micro- and Nano-Scale Technologies in Life Sciences II | Celebration 4 |
| Tuesday | 3:30 PM | 391 | Biomaterials for Immunological Applications* | Celebration 3 |
| Wednesday | 8:00 AM | 447 | Cells, Organs, and Labs on a Chip: Tissue Microenvironments | Celebration 2 |
| Wednesday | 8:00 AM | 466 | Mammalian Synthetic Biology* | Celebration 3 |
| Wednesday | 8:00 AM | 486 | Stem Cells and Tissue Engineering | Celebration 1 |
| Wednesday | 12:30 PM | 505 | Biomaterials in Industry and the Clinic* | Celebration 16 |
| Wednesday | 12:30 PM | 507 | Cells, Organs, and Labs on a Chip | Celebration 1 |
| Wednesday | 12:30 PM | 521 | Engineering the Tissue and Cell Microenvironment I: Promoting Functionality and Repair | Celebration 14 |
| Wednesday | 12:30 PM | 549 | Systems and Quantitative Biology: Signaling Pathways, Response Networks and Growth* | Celebration 2 |
| Wednesday | 3:30 PM | 582 | Engineering the Tissue and Cell Microenvironment II: Disease Models and Mechanisms | Celebration 2 |
| Wednesday | 3:30 PM | 607 | Protein Engineering | Celebration 1 |
| Wednesday | 3:30 PM | 612 | Systems and Quantitative Biology: Modeling Biological Processes* | Celebration 4 |
| Thursday | 8:00 AM | 625 | Biomaterial Scaffolds for Tissue Engineering* | Celebration 10 |
| Thursday | 8:00 AM | 626 | Biomaterials for Drug Delivery: Controlled Release* | Celebration 14 |
| Thursday | 8:00 AM | 638 | Drug Delivery I | Celebration 2 |
| Thursday | 8:00 AM | 663 | Systems and Quantitative Biology: From Communities to Single Cells* | Celebration 4 |
| Thursday | 12:30 PM | 685 | Drug Delivery II | Celebration 2 |
| Thursday | 12:30 PM | 710 | Systems and Quantitative Biology: Drugs and Small Molecules* | Celebration 4 |
| Thursday | 3:30 PM | 719 | Biomolecular Engineering | Celebration 3 |
| Thursday | 3:30 PM | 722 | Cell Migration | Celebration 4 |
| Thursday | 3:30 PM | 725 | Drug Delivery III | Celebration 2 |
| Thursday | 3:30 PM | 736 | Omics and High-Throughput Technologies | Celebration 1 |

^{*} This session is co-sponsored by one or more programming groups

| Day | Time | Session # | Session Title | Room |
|---------------|--------------|--------------|--|----------------------|
| Sunday | 3:30 PM | 8 | 3D Printing Applications in Catalysts, Reactions, and Energy Industry* | Bayhill 28 |
| Monday | 8:00 AM | 64 | Developments in Catalytic Conversion to Chemicals | Challenger 38/39 |
| Monday | 12:30 PM | 129 | Developments in Electrochemical Reactors, Fuel Cells, and Electrolyzers | Challenger 38/39 |
| Monday | 3:30 PM | 201 | Developments in Petroleum and Biofuels Refining Technologies | Challenger 38/39 |
| Tuesday | 8:00 AM | 258 | Conceptual Process Design in Refining, Petrochemicals and Gas Processing | Challenger 38/39 |
| Tuesday | 12:30 PM | 308 | Advances in Methane Coupling Reaction and Aromatization* | Challenger 41/42 |
| Tuesday | 12:30 PM | 358 | Refining and Petrochemical Plant Modelling and Operations Improvements | Challenger 38/39 |
| Tuesday | 3:30 PM | 390 | Biomass Thermal Deconstruction via Fast Pyrolysis Biorefineries* | Regency Ballroom U |
| Tuesday | 3:30 PM | 398 | Developments in Shale Gas, LNG, CNG, and LPG | Challenger 38/39 |
| Wednesday | 8:00 AM | 459 | Environmentally Friendly Product and Process Development for Sustainability* | Bayhill 18 |
| Wednesday | 8:00 AM | 480 | Properties and Phase Equilibria for Fuels and Petrochemicals I | Challenger 38/39 |
| Wednesday | 12:30 PM | 547 | Properties and Phase Equilibria for Fuels and Petrochemicals II | Challenger 38/39 |
| Wednesday | 3:30 PM | 563 | Poster Session: Fuels and Petrochemicals Division | Regency Ballroom R/S |
| Thursday | 8:00 AM | 636 | Developments in Shale Oil, Oil Sands and Other Heavy Fuels | Challenger 38/39 |
| Thursday | 12:30 PM | 684 | Developments in Alternative Fuels and Enabling Technologies I | Challenger 38/39 |
| Thursday | 3:30 PM | 723 | Developments in Alternative Fuels and Enabling Technologies II | Challenger 38/39 |
| 17 - Forest a | nd Plant Bio | products Div | rision | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 44 | Value-Added Uses of Industrial Coproducts in Sustainable Uses | Discovery 47 |
| Monday | 8:00 AM | 54 | Biomaterials from Lignocellulosics | Discovery 47 |
| Monday | 12:30 PM | 116 | Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries | Discovery 47 |
| Monday | 3:30 PM | 188 | Poster Session: Novel Products from Forest and Plant Biomass | Regency Ballroom R/S |
| Tuesday | 8:00 AM | 252 | Biomass Characterization, Pretreatment, and Fractionation | Discovery 47 |
| Tuesday | 12:30 PM | 319 | Chemical Modifications and Processing of Biomaterials | Discovery 47 |
| Tuesday | 3:30 PM | 413 | Lignin for Sustainable Industrial Uses | Discovery 47 |
| Wednesday | 8:00 AM | 449 | Chemical Transformations of Lignocellulosics to Fuels and Nanomaterials | Discovery 47 |
| Wednesday | 12:30 PM | 552 | Thermochemical Conversions of Lignins and Lignocellulosics | Discovery 47 |
| Wednesday | 3:30 PM | 613 | Thermochemical Conversion of Biomass | Discovery 47 |
| Thursday | 8:00 AM | 660 | Separation Processes in Biorefineries | Discovery 47 |
| Thursday | 12:30 PM | 669 | Advanced Biomass Conversion Technologies | Discovery 47 |



3:30 PM

717

Thursday

Advances in Lignin Degradation Strategies

Discovery 47

^{*} This session is co-sponsored by one or more programming groups

| 18 - Liaison I | Functions | | | |
|----------------|--------------------|--------------|--|-----------------------------------|
| Day | Time | Session # | Session Title | Room |
| Monday | 11:15 AM | 108 | Presidential Lecture | Plaza International Ballroom H |
| Tuesday | 8:00 AM | 268 | IACChE's James Y. Oldshue Lecture (Invited Talks) | Plaza International Ballroom H |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G |
| Wednesday | 6:00 PM | 615 | William R. Schowalter Lecture | Plaza International Ballroom H |
| 18A - Miscel | laneous | | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 12:30 PM | 775 | AICHE K-12 STEM Showcase & STEM Outreach Competition | Regency Ballroom U |
| Wednesday | 8:00 AM | 781 | The National Academies of Sciences, Engineering, and Medicine Town Hall: Chemical Engineering in the 21st Century | Florida Ballroom C |
| Wednesday | 12:30 PM | 516 | Data Science Education in Chemical Engineering Panel Discussion | Manatee Spring I |
| Wednesday | 3:30 PM | 571 | CACHE 50th Anniversary: The Future of Cyber-Assisted Chemical Engineering Education | Regency Ballroom T |
| 18B - Public | Affairs and I | nformation (| Committee (PAIC) | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:00 PM | 7 | Public Affairs and AIChE: A PAIC Town Hall | Orlando Ballroom M |
| 18C - Young | Professiona | ls Committe | e (YPC) | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 10:00 AM | 4 | Workshop: Career Planning for Prospective Faculty* | Rock Spring I/II |
| Sunday | 3:30 PM | 33 | Panel Discussion: Chemical Process and Product Design Careers in Industry & Academia (Invited Talks)* | Bayhill 17 |
| Sunday | 3:30 PM | 46 | Workshop: Effective Teaching for New or Prospective Faculty* | Rock Spring I/II |
| Sunday | 4:15 PM | 3 | Chemical Engineering in Sustainability (YCOSST) and Policy (WISE) Award Recipient Talks (Invited Talks) | Orlando Ballroom M |
| Monday | 8:00 AM | 83 | Managing in the High Tech World* | Bayhill 18 |
| Monday | 8:00 AM | 100 | Student Paper Competition in Sensor Technology I* | Celebration 10 |
| Monday | 8:00 AM | 105 | Undergraduate Research Presentations - Chemicals & Environment | Bayhill 31 |
| Monday | 12:30 PM | 141 | Exploring Ethical Dilemmas in the Workplace: Workshop* | Bayhill 18 |
| Monday | 12:30 PM | 163 | Student Paper Competition in Sensor Technology II* | Celebration 10 |
| Monday | 12:30 PM | 232 | Undergraduate Research Presentations - Materials and Biotechnology | Bayhill 31 |
| Monday | 3:30 PM | 170 | Undergraduate Research Presentations - Energy and Petrochemicals | Bayhill 31 |
| Monday | 3:30 PM | 212 | How to Prepare Yourself for Management* | Bayhill 18 |
| Tuesday | 8:00 AM | 297 | Tutorial Session on Electrochemical Methods, Systems and Applications (Invited Talks)* | Plaza International Ballroom I |
| Tuesuay | | 1 | What to Expect Moving from Graduate School to Your Future | Bayhill 32 |
| Tuesday | 8:00 AM | 299 | What to Expect moving from Graduate School to four Future | ., |
| | 8:00 AM 8:00 AM | 300 | Woman Chemical Engineers: Managing to Retain Them* | Bayhill 18 |
| Tuesday | - | | | · · |

^{*} This session is co-sponsored by one or more programming groups

| Wednesday | 8:00 AM | 493 | Young Faculty Forum (Invited Talks)* | Bayhill 29/30 |
|----------------|---------------|--------------|--|-----------------------------------|
| Wednesday | 12:30 PM | 516 | Data Science Education in Chemical Engineering Panel Discussion* | Manatee Spring I |
| 18D - Publica | ation Comm | ittee | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 1:30 PM | 171 | Getting Your Research Published (Invited Talks) | Rainbow Spring I/II |
| Monday | 3:30 PM | 173 | Negotiation and Evaluating a Job Offer for Nerds | Orlando Ballroom L |
| Monday | 4:45 PM | 234 | Engineers Can Do Anything: Explore Your Passions and Catalyze Your Potential to Create Your Unicorn Career | Orlando Ballroom L |
| Tuesday | 3:30 PM | 386 | AIChE Journal Futures: New Directions in Chemical Engineering Research (Invited Talks) | Rainbow Spring I/II |
| 18E - Awards | Committee | | | |
| Day | Time | Session # | Session Title | Room |
| Monday | 6:00 PM | 236 | D.I.C. Wang Award Lecture | Regency Ballroom V |
| Tuesday | 11:15 AM | 305 | Andreas Acrivos Award for Professional Progress in Chemical Engineering Lecture | Plaza International Ballroom H |
| Tuesday | 6:00 PM | 434 | SBE's James E. Bailey Award Lecture | Regency Ballroom V |
| Wednesday | 11:15 AM | 495 | John M. Prausnitz AIChE Institute Lecture | Plaza International Ballroom H |
| 18G - Societa | al Impact Op | erating Cou | ncil (SIOC) | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 106 | Unconscious Bias in Engineering: Why Is It Relevant to the Profession and What Can We Do About It?* | Bayhill 26 |
| Tuesday | 8:00 AM | 261 | DORIC: Supporting Our Students with Disabilities* | Bayhill 31 |
| 18H - Licensi | ng and Prof | essional Dev | relopment Committee | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 5:00 PM | 48 | Order of the Engineer | Plaza International Ballroom I |
| 18I - Minority | / Affairs Cor | nmittee (MA | c) | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 106 | Unconscious Bias in Engineering: Why Is It Relevant to the Profession and What Can We Do About It?* | Bayhill 26 |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering | Regency Ballroom C |
| Monday | 5:30 PM | 235 | MAC Eminent Engineers Awards Ceremony | Regency Ballroom C |
| Tuesday | 8:00 AM | 244 | Advancing into Academic Leadership* | Plaza International Ballroom K |
| Tuesday | 11:00 AM | 303 | MAC/MFF Real Talk: Navigating the Academic Career Path to Tenure (Ticketed Event) | Gulf |
| Tuesday | 2:00 PM | 368 | The Current State of STEM Inclusion in the Workplace* | Bayhill 23 |
| 18J - Researd | ch and New | Technology | Committee (RANTC) | |
| Day | Time | Session # | Session Title | Room |
| | 8:00 AM | 269 | Industry 4.0 and Digital Transformation (Invited Talks)* | Bayhill 27 |

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| 18L - Interna | tional Comr | nittee | | |
|----------------------|--------------|---------------|---|-----------------------------------|
| Day | Time | Session # | Session Title | Room |
| Wednesday | 12:30 PM | 520 | Emerging Junior Investigator Open Innovation Forum (Invited Talks) | Celebration 10 |
| Wednesday | 3:30 PM | 588 | KIChE-US Chapter Open Forum (Invited Talks) | Celebration 10 |
| 18M - Wome | n in Chemic | al Engineerir | ng Committee (WIC) | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 9:00 AM | 1 | Undergraduate Professional Workshop for Women & Minorities - hosted by Women in Chemical Engineering (Ticketed Event) | Barrel Spring I |
| Sunday | 9:00 AM | 2 | Women in Chemical Engineering (WIC) presents "Elevating Your Career for Graduate Students and Young Professionals" (Ticketed Event) | Barrel Spring II |
| Monday | 8:00 AM | 91 | Overcoming Hurdles for Women in Innovation and Entrepreneurship | Orlando Ballroom N |
| Monday | 8:00 AM | 106 | Unconscious Bias in Engineering: Why Is It Relevant to the Profession and What Can We Do About It?* | Bayhill 26 |
| Monday | 11:00 AM | 107 | Networking Luncheon -Sponsored by WIC (Women in Chemical Engineering) (Ticketed Event) | Windermere Ballroom X |
| Monday | 3:30 PM | 219 | Panel Discussion: Advice and Mentorship from Female Leaders in Innovation and Entrepreneurship (Invited Talks) | Orlando Ballroom N |
| Tuesday | 8:00 AM | 244 | Advancing into Academic Leadership | Plaza International Ballroom K |
| Tuesday | 8:00 AM | 300 | Woman Chemical Engineers: Managing to Retain Them* | Bayhill 18 |
| Tuesday | 12:30 PM | 310 | AIChE Management Award Recipient Presentation Session: Focusing on Technology and Innovation Management* | Florida Ballroom C |
| Tuesday | 2:00 PM | 368 | The Current State of STEM Inclusion in the Workplace* | Bayhill 23 |
| 180 - Desig n | Institute fo | r Physical Pr | operties (DIPPR) | |
| Day | Time | Session # | Session Title | Room |
| Thursday | 8:00 AM | 664 | Thermodynamics Needs of the Chemical Industry* | Silver Spring I/II |
| 18P - Climate | e Solutions | | | |
| Day | Time | Session # | Session Title | Room |
| Tuesday | 3:30 PM | 395 | Climate Solutions | Silver Spring I/II |
| 20 - Catalysi | s and React | ion Engineer | ing Division | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 8 | 3D Printing Applications in Catalysts, Reactions, and Energy Industry* | Bayhill 28 |
| Sunday | 3:30 PM | 12 | Advances in Enzymatic Catalysis | Florida Ballroom A |
| Sunday | 3:30 PM | 35 | Pyrolysis of Biomass | Plaza International Ballroom E |
| Sunday | 3:30 PM | 36 | Rational Catalyst Design I: Support Effects | Plaza International Ballroom D |
| Sunday | 3:30 PM | 37 | Reaction Engineering for Combustion and Pyrolysis | Plaza International Ballroom F |
| Sunday | 3:30 PM | 38 | Reaction Path Analysis Using Advanced Data Science Methods* | Peacock Spring |
| Monday | 8:00 AM | 58 | Catalysis with Microporous and Mesoporous Materials I: Gas-Phase Reactions | Florida Ballroom A |
| Monday | 8:00 AM | 60 | Combustion Kinetics and Emissions | Plaza International Ballroom F |
| Monday | 8:00 AM | 64 | Developments in Catalytic Conversion to Chemicals* | Challenger 38/39 |

^{*} This session is co-sponsored by one or more programming groups

| Monday | 8:00 AM | 81 | In Honor of Fabio H. Ribeiro's 60th Birthday (Invited Talks) | Florida Ballroom B |
|---------|----------|-----|--|-----------------------------------|
| Monday | 8:00 AM | 88 | Multiphase & Liquid Phase Reaction Engineering | Plaza International Ballroom E |
| Monday | 8:00 AM | 93 | Rational Catalyst Design II: Tuning Performance with Intermetallics, Bimetallics, and Alloys | Plaza International Ballroom D |
| Monday | 12:30 PM | 119 | Catalysis with Microporous and Mesoporous Materials II: Liquid-Phase Reactions | Florida Ballroom A |
| Monday | 12:30 PM | 143 | Fundamentals of Catalysis I | Plaza International Ballroom D |
| Monday | 12:30 PM | 147 | In Honor of the 2018 R.H. Wilhelm Award Winner I (Invited Talks) | Florida Ballroom B |
| Monday | 12:30 PM | 150 | Modeling and Analysis of Chemical Reactors I: Steady-State Behavior | Plaza International Ballroom F |
| Monday | 12:30 PM | 156 | Plenary: Topical Conference in Molecular and Materials Data Science* | Peacock Spring |
| Monday | 12:30 PM | 159 | Reaction Chemistry and Engineering I: From Reaction Mechanisms to Continuous Synthesis | Plaza International Ballroom E |
| Monday | 3:30 PM | 196 | Catalysis with Microporous and Mesoporous Materials III: Material Design | Florida Ballroom A |
| Monday | 3:30 PM | 205 | Electronic Structure Tuning in Catalysis | Florida Ballroom C |
| Monday | 3:30 PM | 208 | Fundamentals of Catalysis II: C1 Chemistry | Plaza International Ballroom D |
| Monday | 3:30 PM | 213 | In Honor of Ruth Baltus II (Invited Talks)* | Barrel Spring I |
| Monday | 3:30 PM | 214 | In Honor of the 2018 R.H. Wilhelm Award Winner II (Invited Talks) | Florida Ballroom B |
| Monday | 3:30 PM | 216 | Modeling and Analysis of Chemical Reactors II: The Impact of Dynamics on Reactor Design | Plaza International Ballroom F |
| Monday | 3:30 PM | 224 | Reaction Chemistry and Engineering II: Catalysis and Process Intensification | Plaza International Ballroom E |
| Tuesday | 8:00 AM | 246 | Applications of Data Science in Catalysis and Reaction Engineering I* | Peacock Spring |
| Tuesday | 8:00 AM | 253 | Breakthroughs in C1 to Chemicals and Processing Engineering* | Regency Ballroom Q |
| Tuesday | 8:00 AM | 265 | Fundamentals of Catalysis III: Hydrogenation and Dehydrogenation | Plaza International Ballroom D |
| Tuesday | 8:00 AM | 270 | In Honor of Dan Luss' 80th Birthday (Invited Talks) | Florida Ballroom B |
| Tuesday | 8:00 AM | 275 | In Recognition of the 50th Anniversary of ExxonMobil Corporate Strategic Research: CRE (Invited Talks) | Rainbow Spring I/II |
| Tuesday | 8:00 AM | 283 | Microreaction Engineering | Plaza International Ballroom E |
| Tuesday | 8:00 AM | 286 | Oxygen and Hydrogen Photocatalysis and Electrocatalysis I | Florida Ballroom A |
| Tuesday | 8:00 AM | 291 | Reaction Path Analysis | Plaza International Ballroom F |
| Tuesday | 12:30 PM | 308 | Advances in Methane Coupling Reaction and Aromatization* | Challenger 41/42 |
| Tuesday | 12:30 PM | 337 | In Honor of Guy Marin's 65th Birthday (Invited Talks) | Florida Ballroom B |
| Tuesday | 12:30 PM | 351 | Multi-Scale Modeling | Plaza International Ballroom F |
| Tuesday | 12:30 PM | 353 | Oxygen and Hydrogen Photocatalysis and Electrocatalysis II | Florida Ballroom A |
| Tuesday | 12:30 PM | 360 | Technology Transfer and Industrial-Academic Interfaces | Plaza International Ballroom E |
| Tuesday | 12:30 PM | 363 | Thermochemical CO ₂ Reduction I: C1 Products | Plaza International Ballroom D |

^{*} This session is co-sponsored by one or more programming groups

| Tuesday | 3:30 PM | 406 | Fundamentals of Computational and Experimental Catalysis | Plaza International Ballroom F |
|-----------|----------|-----|---|-----------------------------------|
| Tuesday | 3:30 PM | 409 | In Honor of Yannis Kevrekidis' 60th Birthday (Invited Talks) | Florida Ballroom B |
| Tuesday | 3:30 PM | 419 | Oxygen and Hydrogen Photocatalysis and Electrocatalysis III | Florida Ballroom A |
| Tuesday | 3:30 PM | 424 | Reaction Engineering Perspectives for Process Intensification from Industry and Academia (Invited Talks) | Plaza International Ballroom E |
| Tuesday | 3:30 PM | 425 | Thermochemical CO ₂ Reduction II: C2+ Chemicals | Plaza International Ballroom D |
| Tuesday | 3:30 PM | 426 | The Role of Solvents in Biomass Upgrading | Florida Ballroom C |
| Wednesday | 8:00 AM | 443 | Applications of Data Science in Catalysis and Reaction Engineering II* | Peacock Spring |
| Wednesday | 8:00 AM | 446 | Catalysis for Nitrogen Chemistry I: Electrocatalytic Nitrogen Reduction | Plaza International Ballroom D |
| Wednesday | 8:00 AM | 461 | Heterogeneous Catalysis in Liquid Media I | Florida Ballroom A |
| Wednesday | 8:00 AM | 464 | In Honor of the 2019 Practice Award Winner (Invited Talks) | Florida Ballroom B |
| Wednesday | 8:00 AM | 474 | New Methods and Developments in Computational Catalysis I | Plaza International Ballroom F |
| Wednesday | 8:00 AM | 476 | Novel Nanoparticles and Nanostructured Materials for Catalysis* | Bayhill 19 |
| Wednesday | 8:00 AM | 481 | Reaction Engineering in Pharmaceuticals and Fine Chemicals | Plaza International Ballroom E |
| Wednesday | 12:30 PM | 506 | Catalysis for Nitrogen Chemistry II: Plasma-Enhanced and Other Non-Thermal Approaches for N_2 Activation | Plaza International Ballroom D |
| Wednesday | 12:30 PM | 519 | Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions I* | Plaza International Ballroom I |
| Wednesday | 12:30 PM | 530 | Heterogeneous Catalysis in Liquid Media II | Florida Ballroom A |
| Wednesday | 12:30 PM | 532 | In Honor of Anthony Dixon's 65th Birthday (Invited Talks) | Florida Ballroom B |
| Wednesday | 12:30 PM | 538 | New Methods and Developments in Computational Catalysis II | Plaza International Ballroom F |
| Wednesday | 12:30 PM | 542 | Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries | Plaza International Ballroom E |
| Wednesday | 12:30 PM | 544 | Practical Applications of Computational Chemistry and Molecular Simulation I* | Rock Spring I/II |
| Wednesday | 3:30 PM | 560 | Poster Session: Catalysis and Reaction Engineering (CRE) Division | Regency Ballroom R/S |
| Thursday | 8:00 AM | 629 | Catalysis for Biomass Upgrading I: Reaction Fundamentals | Florida Ballroom B |
| Thursday | 8:00 AM | 630 | Catalytic Hydrocarbon Processing I: Methane | Plaza International Ballroom E |
| Thursday | 8:00 AM | 632 | Confluence of Experimental and Theoretical Methods | Plaza International Ballroom F |
| Thursday | 8:00 AM | 639 | Electrocatalytic Activation and Conversion of N ₂ , NH ₃ , and CO ₂ | Plaza International Ballroom D |
| Thursday | 8:00 AM | 641 | Green Chemical Reaction Engineering for Sustainability | Florida Ballroom A |
| Thursday | 8:00 AM | 654 | Polymer Reaction Engineering* | Celebration 5 |
| Thursday | 12:30 PM | 678 | Catalysis for Biomass Upgrading II: Novel Catalytic Materials | Florida Ballroom B |
| Thursday | 12:30 PM | 679 | Catalytic Hydrocarbon Processing II: Ethane, Propane, and Light Hydrocarbons | Plaza International Ballroom E |
| Thursday | 12:30 PM | 682 | Deoxygenation and Oxidation in Biomass Upgrading | Plaza International Ballroom F |
| Thursday | 12:30 PM | 686 | Electrochemical CO ₂ Reduction I: Fuels | Plaza International Ballroom D |

^{*} This session is co-sponsored by one or more programming groups

| Thursday | 12:30 PM | 689 | Fundamentals of Surface Chemistry I | Florida Ballroom A |
|---|---|--|---|---|
| Thursday | 12:30 PM | 704 | Practical Applications of Computational Chemistry and Molecular Simulation II* | Rock Spring I/II |
| Thursday | 3:30 PM | 720 | Catalysis for Biomass Upgrading III: Novel Conversion Strategies | Florida Ballroom B |
| Thursday | 3:30 PM | 721 | Catalytic Hydrocarbon Processing III: Fundamentals of Alkane Activation | Plaza International Ballroom E |
| Thursday | 3:30 PM | 726 | Electrochemical CO ₂ Reduction II: Chemicals | Plaza International Ballroom D |
| Thursday | 3:30 PM | 727 | Fundamentals of Surface Chemistry II | Florida Ballroom A |
| Thursday | 3:30 PM | 741 | Reaction Engineering for Biomass Conversion | Plaza International Ballroom F |
| Friday | 8:00 AM | 754 | Elucidating Catalyst Structures Through Advanced Characterization | Celebration 16 |
| Friday | 8:00 AM | 755 | Environmental and Automotive Catalysis I | Celebration 4 |
| Friday | 8:00 AM | 758 | Novel Active Phases in Catalyst Design I: Earth Abundant Metals | Celebration 5 |
| Friday | 8:00 AM | 759 | Photocatalysis and Electrocatalysis I | Celebration 15 |
| Friday | 8:00 AM | 760 | Syngas Production and Gas-to-Liquids Technology | Celebration 6 |
| Friday | 12:30 PM | 762 | Environmental and Automotive Catalysis II | Celebration 4 |
| Friday | 12:30 PM | 765 | Novel Active Phases in Catalyst Design II: Noble Metals | Celebration 5 |
| Friday | 12:30 PM | 766 | Photocatalysis and Electrocatalysis II | Celebration 15 |
| Friday | 12:30 PM | 768 | Reactions in Near-Critical and Supercritical Fluids | Celebration 6 |
| Friday | 12:30 PM | 771 | The Science of Catalyst Synthesis and Processing | Celebration 16 |
| 21 - Compu | tational Mole | cular Scienc | e and Engineering Forum | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 13 | Atomistic and Molecular Modeling and Simulation of Polymers* | Celebration 8 |
| Cunday | | | | |
| Sunday | 3:30 PM | 38 | Reaction Path Analysis Using Advanced Data Science Methods* | Peacock Spring |
| - | 3:30 PM 8:00 AM | 38 50 | Reaction Path Analysis Using Advanced Data Science Methods* Applications of Molecular Modeling to Study Interfacial Phenomena I | Peacock Spring Rock Spring I/II |
| Monday | | | | - |
| Monday Monday | 8:00 AM | 50 | Applications of Molecular Modeling to Study Interfacial Phenomena I | Rock Spring I/II |
| Sunday Monday Monday Monday Monday | 8:00 AM 8:00 AM | 50 73 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* | Rock Spring I/II Peacock Spring |
| Monday Monday Monday | 8:00 AM 8:00 AM 8:00 AM | 50 73 89 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* | Rock Spring I/II Peacock Spring Celebration 15 |
| Monday Monday Monday Monday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM | 50 73 89 124 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 |
| Monday Monday Monday Monday Monday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM | 50 73 89 124 156 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring |
| Monday Monday Monday Monday Monday Monday Monday Monday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM | 50 73 89 124 156 161 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II |
| Monday Monday Monday Monday Monday Monday Monday Monday Monday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM 12:30 PM | 50 73 89 124 156 161 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)* | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II Silver Spring I/II |
| Monday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM 12:30 PM 12:30 PM 3:30 PM | 50 73 89 124 156 161 162 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)* Applications of Data Science in Molecular Sciences I* | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II Silver Spring I/II Peacock Spring |
| Monday Monday Monday Monday Monday Monday Monday Monday Tuesday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM 12:30 PM 12:30 PM 3:30 PM | 50 73 89 124 156 161 162 195 225 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)* Applications of Data Science in Molecular Sciences I* Recent Advances in Molecular Simulation Methods I | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II Silver Spring I/II Peacock Spring Rock Spring I/II |
| Monday Monday Monday Monday Monday Monday Monday Monday Tuesday Tuesday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM | 50 73 89 124 156 161 162 195 225 246 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)* Applications of Data Science in Molecular Sciences I* Recent Advances in Molecular Simulation Methods I Applications of Data Science in Catalysis and Reaction Engineering I* | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II Silver Spring I/II Peacock Spring Rock Spring I/II Peacock Spring Rock Spring I/II |
| Monday Monday Monday Monday Monday Monday Monday Tuesday Tuesday Tuesday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM | 50 73 89 124 156 161 162 195 225 246 247 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)* Applications of Data Science in Molecular Sciences I* Recent Advances in Molecular Simulation Methods I Applications of Data Science in Catalysis and Reaction Engineering I* Applications of Molecular Modeling to Study Interfacial Phenomena II | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II Silver Spring I/II Peacock Spring Rock Spring I/II Peacock Spring Rock Spring I/II |
| Monday Monday Monday Monday Monday Monday Monday Monday Tuesday Tuesday Tuesday Tuesday Tuesday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM 8:00 AM | 50 73 89 124 156 161 162 195 225 246 247 323 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)* Applications of Data Science in Molecular Sciences I* Recent Advances in Molecular Simulation Methods I Applications of Data Science in Catalysis and Reaction Engineering I* Applications of Molecular Modeling to Study Interfacial Phenomena II Data-Driven Design and Modeling of Biomaterials* Industrial Applications of Computational Chemistry and Molecular Simulation | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II Silver Spring I/II Peacock Spring Rock Spring I/II Peacock Spring Rock Spring I/II Peacock Spring Rock Spring |
| Monday Monday Monday Monday Monday | 8:00 AM 8:00 AM 8:00 AM 12:30 PM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM 8:00 AM 12:30 PM | 50 73 89 124 156 161 162 195 225 246 247 323 338 | Applications of Molecular Modeling to Study Interfacial Phenomena I Faculty Candidates in CoMSEF/Area 1a* Multiscale and Coarse-Grained Modeling of Polymers* Computational Solid State Pharmaceutics* Plenary: Topical Conference in Molecular and Materials Data Science* Software Engineering in and for the Molecular Sciences Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)* Applications of Data Science in Molecular Sciences I* Recent Advances in Molecular Simulation Methods I Applications of Data Science in Catalysis and Reaction Engineering I* Applications of Molecular Modeling to Study Interfacial Phenomena II Data-Driven Design and Modeling of Biomaterials* Industrial Applications of Computational Chemistry and Molecular Simulation (Invited Talks) | Rock Spring I/II Peacock Spring Celebration 15 Celebration 7 Peacock Spring Rock Spring I/II Silver Spring I/II Peacock Spring Rock Spring I/II |

^{*} This session is co-sponsored by one or more programming groups

443

Wednesday

8:00 AM

Applications of Data Science in Catalysis and Reaction Engineering $\ensuremath{\mathsf{II}^*}$

Peacock Spring

| Wednesday | 8:00 AM | 474 | New Methods and Developments in Computational Catalysis I* | Plaza International Ballroom F |
|---|--|---|--|--|
| Wednesday | 8:00 AM | 482 | Recent Advances in Molecular Simulation Methods II | Rock Spring I/II |
| Wednesday | 12:30 PM | 502 | Applications of Data Science in Molecular Sciences II* | Peacock Spring |
| Wednesday | 12:30 PM | 516 | Data Science Education in Chemical Engineering Panel Discussion* | Manatee Spring I |
| Wednesday | 12:30 PM | 544 | Practical Applications of Computational Chemistry and Molecular Simulation I | Rock Spring I/II |
| Wednesday | 3:30 PM | 571 | CACHE 50th Anniversary: The Future of Cyber-Assisted Chemical Engineering Education* | Regency Ballroom T |
| Wednesday | 3:30 PM | 584 | Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks) | Rock Spring I/II |
| Wednesday | 3:30 PM | 590 | Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction* | Silver Spring I/II |
| Thursday | 8:00 AM | 629 | Catalysis for Biomass Upgrading I: Reaction Fundamentals* | Florida Ballroom B |
| Thursday | 8:00 AM | 632 | Confluence of Experimental and Theoretical Methods* | Plaza International Ballroom F |
| Thursday | 8:00 AM | 659 | Recent Advances in Interfacial and Nano Particle Simulation Methods | Rock Spring I/II |
| Thursday | 8:00 AM | 664 | Thermodynamics Needs of the Chemical Industry* | Silver Spring I/II |
| Thursday | 12:30 PM | 678 | Catalysis for Biomass Upgrading II: Novel Catalytic Materials* | Florida Ballroom B |
| Thursday | 12:30 PM | 690 | Gas Hydrates Science and Engineering* | Peacock Spring |
| Thursday | 12:30 PM | 702 | New Frontiers of Molecular Thermodynamics (Invited Talks)* | Silver Spring I/II |
| Thursday | 12:30 PM | 704 | Practical Applications of Computational Chemistry and Molecular Simulation II | Rock Spring I/II |
| Thursday | 3:30 PM | 729 | Making Molecular Simulation a Mainstream Chemical Engineering Tool | Rock Spring I/II |
| Friday | 8:00 AM | 761 | The Industrial Fluid Properties Simulation Challenge | Manatee Spring I |
| Friday | 12:30 PM | 764 | Inverse Design of Soft Materials* | Manatee Spring I |
| 22 - Nanosca | ale Science a | and Enginee | ring Forum | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 40 | Self and Directed Assembly at the Nanoscale | Discovery 45 |
| Monday | 8:00 AM | 104 | Topical Plenary: Microbial Interactions with Biomaterials and Host Cells (Invited Talks)* | Celebration 9 |
| | | | (illivited laiks) | |
| Monday | 8:30 AM | 67 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) | Discovery 45 |
| Monday Monday | 8:30 AM 3:30 PM | | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited | Discovery 45 Regency Ballroom R/S |
| | | 67 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) | , |
| Monday | 3:30 PM | 67 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering | Regency Ballroom R/S |
| Monday Monday | 3:30 PM 3:30 PM | 67 186 212 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* | Regency Ballroom R/S Bayhill 18 |
| Monday Monday Tuesday | 3:30 PM 3:30 PM 8:00 AM | 67 186 212 245 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* Applications in Sensors: Biomedical* | Regency Ballroom R/S Bayhill 18 Celebration 10 |
| Monday Monday Tuesday Tuesday | 3:30 PM 3:30 PM 8:00 AM 8:00 AM | 67 186 212 245 264 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* Applications in Sensors: Biomedical* Functional Nanoparticles* | Regency Ballroom R/S Bayhill 18 Celebration 10 Bayhill 20 |
| Monday Monday Tuesday Tuesday Tuesday | 3:30 PM 3:30 PM 8:00 AM 8:00 AM 12:30 PM | 67 186 212 245 264 312 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* Applications in Sensors: Biomedical* Functional Nanoparticles* Applications in Sensors: Wearables and Environmental* | Regency Ballroom R/S Bayhill 18 Celebration 10 Bayhill 20 Celebration 10 |
| Monday Monday Tuesday Tuesday Tuesday Tuesday | 3:30 PM 3:30 PM 8:00 AM 8:00 AM 12:30 PM 3:30 PM | 67 186 212 245 264 312 429 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* Applications in Sensors: Biomedical* Functional Nanoparticles* Applications in Sensors: Wearables and Environmental* Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks)* | Regency Ballroom R/S Bayhill 18 Celebration 10 Bayhill 20 Celebration 10 Celebration 10 |
| Monday Monday Tuesday Tuesday Tuesday Tuesday Wednesday | 3:30 PM 3:30 PM 8:00 AM 8:00 AM 12:30 PM 3:30 PM 8:00 AM | 67 186 212 245 264 312 429 484 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* Applications in Sensors: Biomedical* Functional Nanoparticles* Applications in Sensors: Wearables and Environmental* Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks)* Sensor Development Platforms* | Regency Ballroom R/S Bayhill 18 Celebration 10 Bayhill 20 Celebration 10 Celebration 10 Celebration 10 |
| Monday Monday Tuesday Tuesday Tuesday Tuesday Wednesday Wednesday | 3:30 PM 3:30 PM 8:00 AM 8:00 AM 12:30 PM 3:30 PM 8:00 AM 12:30 PM | 67 186 212 245 264 312 429 484 528 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* Applications in Sensors: Biomedical* Functional Nanoparticles* Applications in Sensors: Wearables and Environmental* Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks)* Sensor Development Platforms* Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles* | Regency Ballroom R/S Bayhill 18 Celebration 10 Bayhill 20 Celebration 10 Celebration 10 Celebration 10 Bayhill 20 |
| Monday Monday Tuesday Tuesday Tuesday Tuesday Wednesday Wednesday Wednesday | 3:30 PM 3:30 PM 8:00 AM 8:00 AM 12:30 PM 3:30 PM 8:00 AM 12:30 PM 12:30 PM | 67 186 212 245 264 312 429 484 528 536 | Division Plenary: Chemical Engineering Principles for Nanotechnology (Invited Talks) Poster Session: Nanoscale Science and Engineering How to Prepare Yourself for Management* Applications in Sensors: Biomedical* Functional Nanoparticles* Applications in Sensors: Wearables and Environmental* Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks)* Sensor Development Platforms* Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles* Nanofabrication and Nanoscale Processing I | Regency Ballroom R/S Bayhill 18 Celebration 10 Bayhill 20 Celebration 10 Celebration 10 Celebration 10 Bayhill 20 Discovery 45 |

^{*} This session is co-sponsored by one or more programming groups

| Wednesday | 3:30 PM | 598 | Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications* | Bayhill 20 |
|--------------|-------------|-----------|--|--------------------|
| Wednesday | 3:30 PM | 604 | Polymer Thin Films, Nanoconfinement, and Interfaces II* | Celebration 15 |
| Thursday | 3:30 PM | 733 | Nanomaterial Applications for Human Health and the Environment* | Regency Ballroom V |
| Thursday | 3:30 PM | 734 | Nanoscale Phenomena in Macromolecular Systems* | Celebration 5 |
| 22A - Carbo | n Nanomate | rials | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 18 | Carbon Nanofibers and Related Structures from Renewable and/or Cheap Feedstock and Their Applications | Discovery 44 |
| Monday | 12:30 PM | 117 | Carbon Nanomaterials Graduate Student Award Session | Discovery 44 |
| Tuesday | 8:30 AM | 301 | Area Plenary: Carbon Nanomaterials (Invited Talks) | Discovery 44 |
| Tuesday | 12:30 PM | 333 | Graphene 2-D Materials: Synthesis, Functions and Applications I | Discovery 44 |
| Tuesday | 3:30 PM | 407 | Graphene 2-D Materials: Synthesis, Functions and Applications II | Discovery 44 |
| Wednesday | 8:00 AM | 460 | Graphene and Carbon Nanotubes: Absorption, Separations, and Transport Processes | Discovery 44 |
| Wednesday | 12:30 PM | 529 | Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion | Discovery 44 |
| 22B - Bionar | notechnolog | У | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 15 | Biomimetic Materials I* | Celebration 5 |
| Sunday | 3:30 PM | 31 | Nanobiotechnology for Sensors and Imaging I | Discovery 46 |
| Monday | 8:00 AM | 55 | Biomimetic Materials II* | Celebration 5 |
| Monday | 8:00 AM | 104 | Topical Plenary: Microbial Interactions with Biomaterials and Host Cells (Invited Talks)* | Celebration 9 |
| Monday | 12:30 PM | 135 | Emerging Antimicrobial Methods* | Celebration 9 |
| Monday | 12:30 PM | 151 | Nanobiotechnology for Sensors and Imaging II | Discovery 46 |
| Monday | 12:30 PM | 152 | Nanotechnology and 3D Printing: The Intertwined Technologies | Discovery 45 |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research* | Celebration 9 |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 8:00 AM | 249 | Area Plenary: Bionanotechnology (Invited Talks) | Discovery 45 |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 315 | Bionanotechnology Graduate Student Award Session I | Discovery 45 |
| Tuesday | 3:30 PM | 393 | Bionanotechnology Graduate Student Award Session II | Discovery 45 |
| Wednesday | 8:00 AM | 473 | Nanotechnology for Biotechnology and Pharmaceuticals | Discovery 45 |
| Wednesday | 3:30 PM | 609 | Self-Assembled Biomaterials | Discovery 44 |
| Thursday | 8:00 AM | 625 | Biomaterial Scaffolds for Tissue Engineering* | Celebration 10 |
| Thursday | 8:00 AM | 628 | Bionanotechnology for Gene and Drug Delivery I | Discovery 45 |
| Thursday | 8:00 AM | 650 | Nanomaterials for Biological Applications I | Discovery 44 |
| Thursday | 12:30 PM | 676 | Bionanotechnology for Gene and Drug Delivery II | Discovery 45 |
| Thursday | 12:30 PM | 700 | Nanomaterials for Biological Applications II | Discovery 44 |
| Thursday | 3:30 PM | 735 | Nanostructured Biomimetic and Biohybrid Materials and Devices | Discovery 45 |

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| 22C - Nanon | naterials for | Energy Appl | ications | |
|---------------|---------------|-------------|---|--------------------|
| Day | Time | Session # | Session Title | Room |
| Tuesday | 12:30 PM | 352 | Nanomaterials for Energy Storage I: Li-ion and Li Metal Batteries | Discovery 46 |
| Tuesday | 3:30 PM | 418 | Nanomaterials for Hydrogen Production and Fuel Cells I: Fuel Cells | Discovery 46 |
| Wednesday | 8:00 AM | 472 | Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon | Discovery 46 |
| Wednesday | 12:30 PM | 537 | Nanomaterials for Energy Storage II: Supercapacitors | Discovery 46 |
| Wednesday | 3:30 PM | 594 | Nanomaterials for Hydrogen Production and Fuel Cells II: Water-Splitting | Discovery 46 |
| 23 - Sustaina | able Engine | ering Forum | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 24 | Fundamentals of Food, Energy, and Water Systems* | Blue Spring I/II |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering* | Regency Ballroom |
| Monday | 3:30 PM | 205 | Electronic Structure Tuning in Catalysis* | Florida Ballroom C |
| Wednesday | 8:00 AM | 459 | Environmentally Friendly Product and Process Development for Sustainability* | Bayhill 18 |
| Wednesday | 8:00 AM | 487 | Sustainable Engineering Forum Plenary (Invited Talks) | Regency Ballroom |
| 23A - Sustai | nability Scie | nce and Eng | ineering | |
| Day | Time | Session # | Session Title | Room |
| Monday | 8:00 AM | 51 | Big Data and Analytics for Sustainability | Regency Ballroom |
| Monday | 8:00 AM | 80 | Industrial Applications of Integrated Synthesis, Design and Operations Through Modeling and Optimization* | Bayhill 17 |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering* | Regency Ballroom |
| Monday | 12:30 PM | 166 | Sustainable Management and Uses of Post-Consumer Materials and Waste | Regency Ballroom |
| Monday | 3:30 PM | 211 | Green Chemistry and Engineering | Regency Ballroom |
| Tuesday | 12:30 PM | 325 | Design for a Circular Economy | Regency Ballroom |
| Tuesday | 12:30 PM | 361 | The Food-Energy-Water Nexus | Regency Ballroom |
| Tuesday | 12:30 PM | 362 | Thermal Energy Storage* | Bayhill 29/30 |
| Wednesday | 12:30 PM | 511 | Chemical Safety and Sustainability | Regency Ballroom |
| Wednesday | 3:30 PM | 587 | Integrated Process Engineering and Economic Analysis* | Regency Ballroom |
| Thursday | 8:00 AM | 661 | Sustainability and Consumer Products | Regency Ballroom |
| Thursday | 12:30 PM | 687 | Energy Sustainability: Challenges and Solutions | Regency Ballroom |
| Thursday | 12:30 PM | 706 | Process Design: Innovation for Sustainability | Regency Ballroom |
| Thursday | 3:30 PM | 733 | Nanomaterial Applications for Human Health and the Environment | Regency Ballroom |
| Thursday | 3:30 PM | 739 | Process Design in Energy and Sustainability* | Bayhill 26 |
| 23B - Sustai | nable Bioref | fineries | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 12 | Advances in Enzymatic Catalysis* | Florida Ballroom A |
| Sunday | 3:30 PM | 23 | Feedstock Logistics for Biorefineries | Regency Ballroom |
| Sunday | 3:30 PM | 39 | Reactor Engineering for Biomass Feedstocks | Regency Ballroom |
| Sunday | 3:30 PM | 43 | Value-Added Co-Products from Lignin for Biorefineries | Regency Ballroom |
| Monday | 8:00 AM | 70 | Efficient Biological Processing of Lignin to Bioproducts and Biofuels* | Regency Ballroom |
| Monday | 8:00 AM | 82 | Integrating Municipal, Food, and Industrial Waste into Biorefineries | Regency Ballroom |
| Monday | 12:30 PM | 116 | Biochemical Conversion Processes in Forest/Plant Biomass Biorefineries* | Discovery 47 |

^{*} This session is co-sponsored by one or more programming groups

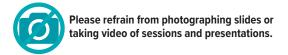
| Monday | 12:30 PM | 134 | Efficient Chemical Processing of Lignin to Bioproducts and Biofuels* | Regency Ballroom Q |
|--|--|---|---|--|
| Monday | 12:30 PM | 157 | Process Innovations on Renewable Polymers and Biobased Intermediates* | Bayhill 17 |
| Monday | 12:30 PM | 164 | Sustainable Biorefineries Plenary Session (Invited Talks) | Regency Ballroom T |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering* | Regency Ballroom O |
| Monday | 3:30 PM | 197 | Chemical and Catalytic Conversions and Processes for Renewable Feedstocks | Regency Ballroom T |
| Tuesday | 8:00 AM | 251 | Biofuels Production: Design, Simulation, and Economic Analysis | Regency Ballroom U |
| Tuesday | 8:00 AM | 252 | Biomass Characterization, Pretreatment, and Fractionation* | Discovery 47 |
| Tuesday | 3:30 PM | 390 | Biomass Thermal Deconstruction via Fast Pyrolysis Biorefineries | Regency Ballroom U |
| Wednesday | 12:30 PM | 497 | Advances in Algal Biorefineries | Regency Ballroom V |
| Wednesday | 12:30 PM | 552 | Thermochemical Conversions of Lignins and Lignocellulosics* | Discovery 47 |
| Wednesday | 3:30 PM | 565 | Poster Session: Sustainability and Sustainable Biorefineries | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 613 | Thermochemical Conversion of Biomass* | Discovery 47 |
| Thursday | 8:00 AM | 624 | Biological Conversions and Processes for Renewable Feedstocks | Regency Ballroom T |
| Thursday | 8:00 AM | 660 | Separation Processes in Biorefineries* | Discovery 47 |
| Thursday | 12:30 PM | 669 | Advanced Biomass Conversion Technologies * | Discovery 47 |
| Thursday | 12:30 PM | 695 | Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals | Regency Ballroom T |
| | | | | |
| Thursday | 3:30 PM | 724 | Developments in Biorefineries | Regency Ballroom T |
| Thursday 23C - Sustair | | | Developments in Biorefineries | Regency Ballroom I |
| , | | | Developments in Biorefineries Session Title | Regency Ballroom I |
| 23C - Sustair | nable Energ | у | | |
| 23C - Sustair Day | nable Energ | y Session # | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply | Room |
| 23C - Sustair Day Monday | Time 8:00 AM | Session # | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply | Room Regency Ballroom V |
| 23C - Sustair Day Monday Monday | Time 8:00 AM 12:30 PM | Session # 62 128 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II | Room Regency Ballroom V Regency Ballroom V |
| 23C - Sustain Day Monday Monday Monday Monday | Time 8:00 AM 12:30 PM 12:30 PM | Session # 62 128 165 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O |
| 23C - Sustair Day Monday Monday Monday Monday Monday Monday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM | Session # 62 128 165 200 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O Regency Ballroom V |
| 23C - Sustain Day Monday Monday Monday Monday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM | Session # 62 128 165 200 215 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* | Room Regency Ballroom V Regency Ballroom O Regency Ballroom V Regency Ballroom V |
| 23C - Sustair Day Monday Monday Monday Monday Monday Tuesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM | Session # 62 128 165 200 215 257 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I | Room Regency Ballroom V Regency Ballroom O Regency Ballroom V Regency Ballroom V Regency Ballroom C |
| 23C - Sustain Day Monday Monday Monday Monday Tuesday Tuesday Tuesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM | Session # 62 128 165 200 215 257 286 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* | Room Regency Ballroom V Regency Ballroom O Regency Ballroom V Regency Ballroom V Regency Ballroom C Regency Ballroom C |
| 23C - Sustain Day Monday Monday Monday Monday Tuesday Tuesday Tuesday Tuesday Tuesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM 8:00 AM | Session # 62 128 165 200 215 257 286 294 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* The Energy-Water Nexus Meet the Innovators: Transforming the Future through Chemical Engineering | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O Regency Ballroom Q Regency Ballroom T Florida Ballroom A Regency Ballroom V Plaza International |
| 23C - Sustain Day Monday Monday Monday Monday Tuesday Tuesday Tuesday Tuesday Tuesday Tuesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM 8:00 AM 11:00 AM | Session # 62 128 165 200 215 257 286 294 304 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* The Energy-Water Nexus Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O Regency Ballroom Q Regency Ballroom T Florida Ballroom A Regency Ballroom V Plaza International Ballroom G |
| 23C - Sustain Day Monday Monday Monday Monday Tuesday Tuesday Tuesday Tuesday Tuesday Tuesday Tuesday Tuesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM 8:00 AM 11:00 AM 12:30 PM | Session # 62 128 165 200 215 257 286 294 304 321 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* The Energy-Water Nexus Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* Concentrated Solar Energy for Power Generation and Chemical Processing II* Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O Regency Ballroom Q Regency Ballroom T Florida Ballroom A Regency Ballroom V Plaza International Ballroom G Regency Ballroom T |
| 23C - Sustain Day Monday Monday Monday Monday Tuesday Tuesday Tuesday Tuesday Tuesday Tuesday Tuesday Tuesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 3:30 PM 8:00 AM 8:00 AM 11:00 AM 12:30 PM | Session # 62 128 165 200 215 257 286 294 304 321 345 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* The Energy-Water Nexus Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* Concentrated Solar Energy for Power Generation and Chemical Processing II* Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Material Innovations* | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O Regency Ballroom Q Regency Ballroom T Florida Ballroom A Regency Ballroom V Plaza International Ballroom G Regency Ballroom T Regency Ballroom T |
| 23C - Sustain Day Monday Monday Monday Monday Monday Tuesday Wednesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 8:00 AM 8:00 AM 11:00 AM 12:30 PM 12:30 PM | Session # 62 128 165 200 215 257 286 294 304 321 345 396 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* The Energy-Water Nexus Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* Concentrated Solar Energy for Power Generation and Chemical Processing II* Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Material Innovations* Concentrated Solar Energy for Power Generation and Chemical Processing III* | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O Regency Ballroom V Regency Ballroom Q Regency Ballroom T Florida Ballroom A Regency Ballroom V Plaza International Ballroom G Regency Ballroom T Regency Ballroom Q Regency Ballroom C |
| 23C - Sustain Day Monday Monday Monday Monday Monday Tuesday | Time 8:00 AM 12:30 PM 12:30 PM 3:30 PM 8:00 AM 8:00 AM 11:00 AM 12:30 PM 12:30 PM 12:30 PM | Session # 62 128 165 200 215 257 286 294 304 321 345 396 525 | Session Title Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II Career Paths: Perspectives by Minority Professionals in Chemical Engineering* Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development* Concentrated Solar for Power Generation and Chemical Processing I Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* The Energy-Water Nexus Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* Concentrated Solar Energy for Power Generation and Chemical Processing II* Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Material Innovations* Concentrated Solar Energy for Power Generation and Chemical Processing III* Fuel and Energy Decarbonization Poster Session: Concentrated Solar Energy for Power Generation and | Room Regency Ballroom V Regency Ballroom V Regency Ballroom O Regency Ballroom V Regency Ballroom T Florida Ballroom A Regency Ballroom V Plaza International Ballroom G Regency Ballroom T Regency Ballroom T Regency Ballroom T |

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| Day Time Session # Session Title | | | | | |
|----------------------------------|--------------|--------------|--|-----------------------------------|--|
| Day | Time | Session # | Session Title | Room | |
| Monday | 12:30 PM | 148 | Intellectual Property for Practicing Engineers: Patents and Trade Secrets | Orlando Ballroom N | |
| Wednesday | 12:30 PM | 508 | Challenges and Best Practices in Technology Commercialization* | Bayhill 18 | |
| 25 - Upstrea | m Engineeri | ng and Flow | Assurance Forum | | |
| Day | Time | Session # | Session Title | Room | |
| Monday | 8:00 AM | 75 | Fundamentals and Applications of Flow Assurance | Challenger 40 | |
| Monday | 12:30 PM | 155 | Phase Behavior and Flow of Reservoir Fluids | Challenger 40 | |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 | |
| Tuesday | 8:00 AM | 274 | Innovations in Production of Unconventional Reservoirs | Challenger 40 | |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 | |
| Tuesday | 12:30 PM | 330 | Flow Assurance and Asset Integrity | Challenger 40 | |
| Tuesday | 3:30 PM | 383 | Poster Session: Upstream Engineering and Flow Assurance | Regency Ballroom R/S | |
| Thursday | 12:30 PM | 690 | Gas Hydrates Science and Engineering* | Peacock Spring | |
| 26 - Pharma | ceutical Dis | covery, Deve | elopment and Manufacturing Forum | | |
| Day | Time | Session # | Session Title | Room | |
| Sunday | 3:30 PM | 11 | Advanced Modelling and Data Systems Applications in Next-Gen Manufacturing* | Bayhill 27 | |
| Sunday | 3:30 PM | 12 | Advances in Enzymatic Catalysis* | Florida Ballroom A | |
| Sunday | 3:30 PM | 42 | Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond* | Coral Spring I/II | |
| Monday | 8:00 AM | 74 | Forum Plenary: Opportunities and Challenges with Journey from Industry 4.0 to Pharma 4.0 | Celebration 6 | |
| Monday | 8:00 AM | 94 | Regenerative Engineering: Substrate-Derived Control of Cellular Behavior* | Celebration 8 | |
| Monday | 12:30 PM | 124 | Computational Solid State Pharmaceutics | Celebration 7 | |
| Monday | 12:30 PM | 125 | Continuous Crystallization Processes* | Coral Spring I/II | |
| Monday | 12:30 PM | 126 | Continuous Processing in Drug Substance | Celebration 6 | |
| Monday | 12:30 PM | 160 | Regenerative Engineering: Stem Cells and Mechanotransduction* | Celebration 8 | |
| Monday | 3:30 PM | 189 | Poster Session: Pharmaceutical | Regency Ballroom R/S | |
| Monday | 3:30 PM | 198 | Crystallization of Pharmaceutical and Biological Molecules* | Coral Spring I/II | |
| Monday | 6:30 PM | 237 | Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony | Regency Ballroom U | |
| Tuesday | 8:00 AM | 240 | Advances in Large Molecule Processes | Celebration 7 | |
| Tuesday | 8:00 AM | 259 | Data Science & Analytics for Operations Support and Predictions in Pharmaceutical Processes & Products | Celebration 6 | |
| Tuesday | 8:00 AM | 260 | Development of Pharmaceutical Process Control Strategies for Drug Product Manufacture | Celebration 8 | |
| Tuesday | 8:00 AM | 284 | Modeling and Control of Crystallization I* | Coral Spring I/II | |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G | |
| Tuesday | 12:30 PM | 322 | Continuous Drug Substance Isolation | Celebration 6 | |
| Tuesday | 12:30 PM | 340 | Innovations in Particle Engineering: From Amorphous Solid Dispersions to New Processing | Celebration 7 | |
| Tuesday | 12:30 PM | 342 | Integrated Design for Drug Substance Synthesis | Celebration 8 | |

^{*} This session is co-sponsored by one or more programming groups

| Tuesday | 12:30 PM | 344 | Machine Learning Applications and Intelligent Systems* | Bayhill 26 |
|-----------|----------|-----|--|-----------------------------------|
| Tuesday | 12:30 PM | 354 | Pharma 4.0 (Invited Talks)* | Bayhill 27 |
| Tuesday | 3:30 PM | 399 | Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)* | Regency Ballroom V |
| Tuesday | 3:30 PM | 410 | Innovations and Emerging Technologies: Drug Substance and Drug Product Development | Celebration 8 |
| Tuesday | 3:30 PM | 421 | Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals I | Celebration 7 |
| Tuesday | 3:30 PM | 423 | Process-wide and Operational Topics | Celebration 6 |
| Wednesday | 8:00 AM | 451 | Continuous Processing Technologies Applied in Drug Product Manufacturing | Celebration 7 |
| Wednesday | 8:00 AM | 470 | Mixing Scale-Up and Scale-Down Issues in Pharmaceutical and Biopharmaceutical Processes* | Bayhill 32 |
| Wednesday | 8:00 AM | 471 | Modeling and Design of Biopharmaceutical Processes | Celebration 8 |
| Wednesday | 8:00 AM | 478 | Panel on Pre-Competitive Collaboration (Invited Talks) | Celebration 6 |
| Wednesday | 8:00 AM | 481 | Reaction Engineering in Pharmaceuticals and Fine Chemicals* | Plaza International Ballroom E |
| Wednesday | 8:00 AM | 492 | Understanding Powder Processing via Materials Science | Celebration 14 |
| Wednesday | 12:30 PM | 496 | 3D Printing in Pharmaceutical and Health Industry* | Bayhill 28 |
| Wednesday | 12:30 PM | 499 | Advances in Drug Discovery Processes | Celebration 7 |
| Wednesday | 12:30 PM | 509 | Characterization of Continuous Drug Product Unit Operations | Celebration 6 |
| Wednesday | 12:30 PM | 516 | Data Science Education in Chemical Engineering Panel Discussion* | Manatee Spring I |
| Wednesday | 12:30 PM | 533 | Integrated Design for Solid Drug Products | Celebration 8 |
| Wednesday | 12:30 PM | 542 | Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries* | Plaza International Ballroom E |
| Wednesday | 3:30 PM | 577 | Development of Pharmaceutical Process Control Strategies for Drug Substance Manufacture | Celebration 8 |
| Wednesday | 3:30 PM | 600 | Particle Engineering and Crystallization in Materials Science | Celebration 6 |
| Wednesday | 3:30 PM | 605 | Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals II | Celebration 7 |
| Thursday | 8:00 AM | 626 | Biomaterials for Drug Delivery: Controlled Release* | Celebration 14 |
| Thursday | 8:00 AM | 640 | Enabling and Advancing Formulations in Drug Product | Celebration 6 |
| Thursday | 8:00 AM | 642 | In-Silico Tools for Accelerating Pharmaceutical Process Development | Celebration 7 |
| Thursday | 8:00 AM | 651 | Particle Formation and Crystallization Processes from Liquids, Slurries, and Emulsions* | Coral Spring I/II |
| Thursday | 12:30 PM | 672 | Big-Data for Process Applications* | Bayhill 26 |
| Thursday | 12:30 PM | 683 | Development of Pharmaceutical Process Control Strategies for Production of Biologics | Celebration 6 |
| Thursday | 12:30 PM | 693 | Innovations and Emerging Technologies: Automated Platforms and Novel Methodologies | Celebration 7 |
| Friday | 8:00 AM | 753 | Data-Driven and Hybrid Modeling for Decision Making* | Celebration 1 |



^{*} This session is co-sponsored by one or more programming groups

| POSTERSESS | SIONS - Post | ter Sessions | | |
|------------|--------------|--------------|---|----------------------|
| Day | Time | Session # | Session Title | Room |
| Sunday | 1:00 PM | 6 | Meet the Faculty and Post-Doc Candidates Poster Session* | Regency Ballroom R/S |
| Monday | 3:30 PM | 174 | General Poster Session I | Regency Ballroom R/S |
| Monday | 3:30 PM | 175 | Poster Session: Bioengineering* | Regency Ballroom R/S |
| Monday | 3:30 PM | 176 | Poster Session: Engineering Fundamentals in Life Science* | Regency Ballroom R/S |
| Monday | 3:30 PM | 177 | Poster Session: Food and Bioprocess Engineering* | Regency Ballroom R/S |
| Monday | 3:30 PM | 178 | Poster Session: Food Innovation and Engineering* | Regency Ballroom R/S |
| Monday | 3:30 PM | 179 | Poster Session: General Poster Session in Sensors* | Regency Ballroom R/S |
| Monday | 3:30 PM | 180 | Poster Session: Interfacial Phenomena (Area 1C)* | Orlando Ballroom M |
| Monday | 3:30 PM | 181 | Poster Session: Materials Engineering & Sciences (08A - Polymers)* | Regency Ballroom R/S |
| Monday | 3:30 PM | 182 | Poster Session: Materials Engineering & Sciences (08B - Biomaterials)* | Regency Ballroom R/S |
| Monday | 3:30 PM | 183 | Poster Session: Materials Engineering & Sciences (08D - Inorganic Materials)* | Regency Ballroom R/S |
| Monday | 3:30 PM | 184 | Poster Session: Materials Engineering & Sciences (08E - Electronic and Photonic Materials)* | Regency Ballroom R/S |
| Monday | 3:30 PM | 185 | Poster Session: Materials Engineering & Sciences (08F - Composite Materials)* | Regency Ballroom R/S |
| Monday | 3:30 PM | 186 | Poster Session: Nanoscale Science and Engineering* | Regency Ballroom R/S |
| Monday | 3:30 PM | 187 | Poster Session: Next-Gen Manufacturing* | Regency Ballroom R/S |
| Monday | 3:30 PM | 188 | Poster Session: Novel Products from Forest and Plant Biomass* | Regency Ballroom R/S |
| Monday | 3:30 PM | 189 | Poster Session: Pharmaceutical* | Regency Ballroom R/S |
| Monday | 3:30 PM | 221 | Poster Session: Fluid Mechanics* | Orlando Ballroom M |
| Tuesday | 3:30 PM | 369 | Interactive Session: Applied Mathematics and Numerical Analysis* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 370 | Interactive Session: Data and Information Systems* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 371 | Interactive Session: Systems and Process Control* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 372 | Interactive Session: Systems and Process Design* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 373 | Interactive Session: Systems and Process Operations* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 374 | Poster Session: Bioseparations* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 375 | Poster Session: Chemical Engineering Education* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 376 | Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 377 | Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 378 | Poster Session: General Topics on Separations* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 379 | Poster Session: In Recognition of the 50th Anniversary of ExxonMobil Corporate Strategic Research | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 380 | Poster Session: Particle Technology Forum* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 381 | Poster Session: Separations Division* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 382 | Poster Session: Thermodynamics and Transport Properties (Area 1A)* | Regency Ballroom R/S |
| Tuesday | 3:30 PM | 383 | Poster Session: Upstream Engineering and Flow Assurance* | Regency Ballroom R/S |
| Tuesday | 6:00 PM | 435 | Poster Session: Ammonia Energy* | Regency Ballroom P |
| Wednesday | 3:30 PM | 558 | General Poster Session II | Regency Ballroom R/S |

^{*} This session is co-sponsored by one or more programming groups

| Wednesday | 3:30 PM | 559 | Poster Session: Advances in Fossil Energy R&D* | Regency Ballroom R/S |
|---------------|--------------|--------------|---|-----------------------------------|
| | | | 3, | |
| Wednesday | 3:30 PM | 560 | Poster Session: Catalysis and Reaction Engineering (CRE) Division* | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 561 | Poster Session: Concentrated Solar Energy for Power Generation and Chemical Processing* | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 562 | Poster Session: Environmental Division* | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 563 | Poster Session: Fuels and Petrochemicals Division* | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 564 | Poster Session: Process Development* | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 565 | Poster Session: Sustainability and Sustainable Biorefineries* | Regency Ballroom R/S |
| Wednesday | 3:30 PM | 566 | Poster Session: Transport and Energy Processes* | Regency Ballroom R/S |
| T1 - Meet the | Faculty and | d Post-Doc C | andidates Poster Session Sponsored by the Education Division | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 10:00 AM | 4 | Workshop: Career Planning for Prospective Faculty* | Rock Spring I/II |
| Sunday | 1:00 PM | 6 | Meet the Faculty and Post-Doc Candidates Poster Session | Regency Ballroom R/S |
| Sunday | 3:30 PM | 14 | Biomaterials and Life Science Engineering: Faculty Candidates I* | Celebration 7 |
| Sunday | 3:30 PM | 46 | Workshop: Effective Teaching for New or Prospective Faculty* | Rock Spring I/II |
| Tuesday | 12:30 PM | 327 | Electrochemical Fundamentals: Faculty Candidate Session* | Plaza International Ballroom J |
| T2 - Entrepre | neurship in | Chemical E | ngineering - Sponsored by CIEE | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 21 | Chemical Angels Network (CAN) Session: Entrepreneurship & Investing in Early-Stage Chemical Companies | Orlando Ballroom N |
| Monday | 8:00 AM | 91 | Overcoming Hurdles for Women in Innovation and Entrepreneurship* | Orlando Ballroom N |
| Monday | 12:30 PM | 148 | Intellectual Property for Practicing Engineers: Patents and Trade Secrets* | Orlando Ballroom N |
| Monday | 3:30 PM | 219 | Panel Discussion: Advice and Mentorship from Female Leaders in Innovation and Entrepreneurship (Invited Talks)* | Orlando Ballroom N |
| Tuesday | 8:00 AM | 328 | Entrepreneurship and Investing in Early Stage Companies | Orlando Ballroom N |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G |
| Tuesday | 12:30 PM | 254 | Challenges in Entrepreneurship: Ensuring Success for your Start-up | Orlando Ballroom N |
| Tuesday | 3:30 PM | 401 | Entrepreneurship in Chemical Engineering: Transitioning from the Lab to the Boardroom | Orlando Ballroom N |
| T3 - Applicat | ions of Data | Science to | Molecules and Materials | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 38 | Reaction Path Analysis Using Advanced Data Science Methods | Peacock Spring |
| Monday | 12:30 PM | 156 | Plenary: Topical Conference in Molecular and Materials Data Science | Peacock Spring |
| Monday | 3:30 PM | 195 | Applications of Data Science in Molecular Sciences I | Peacock Spring |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 |
| Tuesday | 8:00 AM | 246 | Applications of Data Science in Catalysis and Reaction Engineering I | Peacock Spring |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 |
| Tuesday | 12:30 PM | 323 | Data-Driven Design and Modeling of Biomaterials | Peacock Spring |
| Tuesday | 3:30 PM | 411 | Innovations in Methods of Data Science | Peacock Spring |
| | 8:00 AM | | Applications of Data Science in Catalysis and Reaction Engineering II | Peacock Spring |
| Wednesday | 6.00 AW | 443 | Applications of Data Science in Catalysis and Reaction Engineering if | reaction Spring |

 $[\]ensuremath{^{*}}$ This session is co-sponsored by one or more programming groups

| T4 - Concent | T4 - Concentrated Solar Energy for Power Generation and Chemical Processing | | | | |
|---------------|---|-----------|--|-----------------------------------|--|
| Day | Time | Session # | Session Title | Room | |
| Tuesday | 8:00 AM | 257 | Concentrated Solar for Power Generation and Chemical Processing I* | Regency Ballroom T | |
| Tuesday | 8:00 AM | 286 | Oxygen and Hydrogen Photocatalysis and Electrocatalysis I* | Florida Ballroom A | |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G | |
| Tuesday | 12:30 PM | 321 | Concentrated Solar Energy for Power Generation and Chemical Processing II | Regency Ballroom T | |
| Tuesday | 3:30 PM | 396 | Concentrated Solar Energy for Power Generation and Chemical Processing III | Regency Ballroom T | |
| Wednesday | 3:30 PM | 561 | Poster Session: Concentrated Solar Energy for Power Generation and Chemical Processing | Regency Ballroom R/S | |
| Wednesday | 3:30 PM | 591 | Modeling, Control, and Optimization of Energy Systems* | Bayhill 25 | |
| Thursday | 3:30 PM | 745 | Sustainable Energy: Generation and Storage* | Regency Ballroom U | |
| Friday | 8:00 AM | 752 | Applied Math for Energy and Environmental Applications* | Celebration 3 | |
| T5 - Center f | or Hydroger | ı Safety | | | |
| Day | Time | Session # | Session Title | Room | |
| Tuesday | 8:00 AM | 772 | Overview of Hydrogen and Fuel Cell Technologies | Regency Ballroom O | |
| Tuesday | 9:10 AM | 773 | Practicing Hydrogen Safety for Students and Researchers | Regency Ballroom O | |
| T6A - Next-G | en Manufac | turing | | | |
| Day | Time | Session # | Session Title | Room | |
| Sunday | 3:30 PM | 11 | Advanced Modelling and Data Systems Applications in Next-Gen Manufacturing | Bayhill 27 | |
| Sunday | 3:30 PM | 29 | Modeling, Control, and Optimization of Manufacturing Systems* | Bayhill 25 | |
| Monday | 8:00 AM | 52 | Big Data and Data Analytics (Invited Talks) | Bayhill 27 | |
| Monday | 12:30 PM | 130 | Digital Twin (Invited Talks) | Bayhill 28 | |
| Monday | 12:30 PM | 145 | Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond | Bayhill 27 | |
| Monday | 3:30 PM | 187 | Poster Session: Next-Gen Manufacturing | Regency Ballroom R/S | |
| Monday | 3:30 PM | 213 | In Honor of Ruth Baltus II (Invited Talks)* | Barrel Spring I | |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical* | Celebration 10 | |
| Tuesday | 8:00 AM | 269 | Industry 4.0 and Digital Transformation (Invited Talks) | Bayhill 27 | |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental* | Celebration 10 | |
| Tuesday | 12:30 PM | 354 | Pharma 4.0 (Invited Talks) | Bayhill 27 | |
| Tuesday | 3:30 PM | 389 | Artificial Intelligence and Advanced Computation | Bayhill 27 | |
| Wednesday | 8:00 AM | 452 | Cybersecurity | Bayhill 27 | |
| Wednesday | 11:15 AM | 495 | John M. Prausnitz AIChE Institute Lecture* | Plaza International Ballroom H | |
| Wednesday | 12:30 PM | 504 | Big Data and Applications in Advanced Modeling and Manufacturing | Bayhill 27 | |
| Wednesday | 12:30 PM | 516 | Data Science Education in Chemical Engineering Panel Discussion* | Manatee Spring I | |
| Wednesday | 3:30 PM | 570 | Bioprinting of Scaffolds, Tissues, and Organs* | Celebration 12/13 | |
| Wednesday | 3:30 PM | 606 | Process Intensification through Process Systems Engineering* | Bayhill 24 | |
| Wednesday | 3:30 PM | 611 | Sustainable Food Production* | Celebration 9 | |
| Thursday | 8:00 AM | 637 | Distributed Chemical and Energy Processes for Sustainability* | Regency Ballroom U | |
| Thursday | 12:30 PM | 672 | Big-Data for Process Applications* | Bayhill 26 | |

^{*} This session is co-sponsored by one or more programming groups

| Day | Time | Session # | Session Title | Room |
|---------------|-------------|--------------|---|-----------------------------------|
| Monday | 8:00 AM | 92 | Process Intensification and Modular Manufacturing: Modeling and Simulation | Bayhill 28 |
| Monday | 3:30 PM | 213 | In Honor of Ruth Baltus II (Invited Talks)* | Barrel Spring I |
| Tuesday | 8:00 AM | 290 | Process Intensification and Modular Manufacturing: Modular/Advanced Manufacturing | Bayhill 28 |
| Tuesday | 12:30 PM | 357 | Process Intensification and Modular Manufacturing: Fundamentals and Applications | Bayhill 28 |
| Tuesday | 3:30 PM | 390 | Biomass Thermal Deconstruction via Fast Pyrolysis Biorefineries* | Regency Ballroom U |
| Tuesday | 3:30 PM | 422 | Process Research for Improved Throughput & Efficiency, and Reduced Cost* | Bayhill 18 |
| Wednesday | 8:00 AM | 441 | Advances in Process Intensification* | Bayhill 17 |
| Wednesday | 11:15 AM | 495 | John M. Prausnitz AIChE Institute Lecture* | Plaza International Ballroom H |
| Wednesday | 12:30 PM | 545 | Process Intensification By Enhanced Heat and Mass Transfer* | Bayhill 17 |
| Wednesday | 3:30 PM | 606 | Process Intensification through Process Systems Engineering* | Bayhill 24 |
| Thursday | 8:00 AM | 637 | Distributed Chemical and Energy Processes for Sustainability* | Regency Ballroom L |
| Thursday | 8:00 AM | 656 | Process Intensification By Process Integration* | Bayhill 17 |
| Thursday | 12:30 PM | 707 | Process Intensification through the Application of Microreactors, Multiphase Reactors, and Membrane Reactors* | Bayhill 17 |
| T6C - 3D Prir | nting | | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 3:30 PM | 8 | 3D Printing Applications in Catalysts, Reactions, and Energy Industry | Bayhill 28 |
| Monday | 12:30 PM | 152 | Nanotechnology and 3D Printing: The Intertwined Technologies* | Discovery 45 |
| Tuesday | 3:30 PM | 384 | 3D Printing of Composites | Bayhill 28 |
| Wednesday | 8:00 AM | 437 | 3D Printing of Functional Materials | Bayhill 28 |
| Wednesday | 12:30 PM | 496 | 3D Printing in Pharmaceutical and Health Industry | Bayhill 28 |
| Wednesday | 3:30 PM | 567 | 3D Printing Fundamental and Applications | Bayhill 28 |
| Wednesday | 3:30 PM | 568 | Additive Manufacturing of Energetics* | Bayhill 21 |
| Wednesday | 3:30 PM | 570 | Bioprinting of Scaffolds, Tissues, and Organs* | Celebration 12/13 |
| Wednesday | 3:30 PM | 603 | Polymers in Additive Manufacturing | Bayhill 27 |
| T7 - Regener | ative Engin | eering Socie | ty | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 4:15 PM | 3 | Chemical Engineering in Sustainability (YCOSST) and Policy (WISE) Award Recipient Talks (Invited Talks)* | Orlando Ballroom M |
| Monday | 8:00 AM | 94 | Regenerative Engineering: Substrate-Derived Control of Cellular Behavior | Celebration 8 |
| | | | 1 3 | |



 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| T8 - Microbes at Biomedical Interfaces | | | | | |
|--|----------|-----------|--|-----------------------------------|--|
| Day | Time | Session # | Session Title | Room | |
| Monday | 8:00 AM | 104 | Topical Plenary: Microbial Interactions with Biomaterials and Host Cells (Invited Talks) | Celebration 9 | |
| Monday | 12:30 PM | 135 | Emerging Antimicrobial Methods | Celebration 9 | |
| Monday | 3:30 PM | 210 | Graduate Student Competition in Microbiointerface Research | Celebration 9 | |
| Tuesday | 8:00 AM | 293 | Technologies for Understanding Microbial Interactions | Celebration 9 | |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G | |
| Tuesday | 12:30 PM | 316 | Biophysical Properties of Microbes and Microbial Communities | Celebration 9 | |
| Tuesday | 3:30 PM | 428 | Topical Plenary: Fundamentals of Microbial Interactions with Interfaces (Invited Talks) | Celebration 9 | |
| T9 - Sensors | | | | | |
| Day | Time | Session # | Session Title | Room | |
| Sunday | 3:30 PM | 31 | Nanobiotechnology for Sensors and Imaging I* | Discovery 46 | |
| Monday | 8:00 AM | 52 | Big Data and Data Analytics (Invited Talks)* | Bayhill 27 | |
| Monday | 8:00 AM | 100 | Student Paper Competition in Sensor Technology I | Celebration 10 | |
| Monday | 12:30 PM | 109 | Advances in Biosensors and Biodiagnostics: Biosensor and Biodiagnostic Detection Methods* | Celebration 4 | |
| Monday | 12:30 PM | 145 | Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond* | Bayhill 27 | |
| Monday | 12:30 PM | 151 | Nanobiotechnology for Sensors and Imaging II* | Discovery 46 | |
| Monday | 12:30 PM | 163 | Student Paper Competition in Sensor Technology II | Celebration 10 | |
| Monday | 3:30 PM | 179 | Poster Session: General Poster Session in Sensors | Regency Ballroom R/S | |
| Tuesday | 8:00 AM | 245 | Applications in Sensors: Biomedical | Celebration 10 | |
| Tuesday | 8:00 AM | 269 | Industry 4.0 and Digital Transformation (Invited Talks)* | Bayhill 27 | |
| Tuesday | 8:00 AM | 293 | Technologies for Understanding Microbial Interactions * | Celebration 9 | |
| Tuesday | 11:00 AM | 304 | Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)* | Plaza International Ballroom G | |
| Tuesday | 12:30 PM | 306 | Advances in Biosensors and Biodiagnostics: Systems and Devices for Advanced Biosensing* | Celebration 3 | |
| Tuesday | 12:30 PM | 312 | Applications in Sensors: Wearables and Environmental | Celebration 10 | |
| Tuesday | 3:30 PM | 389 | Artificial Intelligence and Advanced Computation* | Bayhill 27 | |
| Tuesday | 3:30 PM | 429 | Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks) | Celebration 10 | |
| Wednesday | 8:00 AM | 484 | Sensor Development Platforms | Celebration 10 | |
| TB - Food Innovation and Engineering | | | | | |
| Day | Time | Session # | Session Title | Room | |
| Sunday | 3:30 PM | 17 | Biotechnological Production of Food and Feed Ingredients* | Celebration 1 | |
| Sunday | 3:30 PM | 24 | Fundamentals of Food, Energy, and Water Systems* | Blue Spring I/II | |
| Monday | 8:00 AM | 82 | Integrating Municipal, Food, and Industrial Waste into Biorefineries* | Regency Ballroom U | |
| Monday | 3:30 PM | 177 | Poster Session: Food and Bioprocess Engineering* | Regency Ballroom R/S | |
| Monday | 3:30 PM | 178 | Poster Session: Food Innovation and Engineering | Regency Ballroom R/S | |
| Tuesday | 8:00 AM | 279 | Membrane Technology in Food and Bioprocess Engineering* | Celebration 1 | |
| Tuesday | 12:30 PM | 347 | Microbiomes and Metabolomes in Food, Health, and Bioprocessing* | Celebration 1 | |

^{*} This session is co-sponsored by one or more programming groups

| Tuesday | 12:30 PM | 361 | The Food-Energy-Water Nexus* | Regency Ballroom V |
|--------------|---------------|-----------|--|-----------------------------------|
| Tuesday | 3:30 PM | 399 | Division Plenary: Food, Pharmaceutical, and Bioengineering Division (Invited Talks)* | Regency Ballroom V |
| Wednesday | 8:00 AM | 491 | Transport Phenomena, Rheology, and Mixing in Food Processing and Engineering (Invited Talks) | Celebration 9 |
| Wednesday | 12:30 PM | 523 | Fermented Food and Beverages | Celebration 9 |
| Wednesday | 3:30 PM | 611 | Sustainable Food Production | Celebration 9 |
| Thursday | 8:00 AM | 655 | Process Engineering in Food and Bioprocess Industries* | Celebration 1 |
| TC - Enginee | ring for Incl | usion | | |
| Day | Time | Session # | Session Title | Room |
| Sunday | 9:00 AM | 1 | Undergraduate Professional Workshop for Women & Minorities - hosted by Women in Chemical Engineering (Ticketed Event)* | Barrel Spring I |
| Sunday | 9:00 AM | 2 | Women in Chemical Engineering (WIC) presents "Elevating Your Career for Graduate Students and Young Professionals" (Ticketed Event)* | Barrel Spring II |
| Sunday | 3:00 PM | 7 | Public Affairs and AIChE: A PAIC Town Hall* | Orlando Ballroom M |
| Monday | 8:00 AM | 91 | Overcoming Hurdles for Women in Innovation and Entrepreneurship* | Orlando Ballroom N |
| Monday | 8:00 AM | 106 | Unconscious Bias in Engineering: Why Is It Relevant to the Profession and What Can We Do About It? | Bayhill 26 |
| Monday | 11:00 AM | 107 | Networking Luncheon -Sponsored by WIC (Women in Chemical Engineering) (Ticketed Event)* | Windermere Ballroon |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering* | Regency Ballroom O |
| Monday | 3:30 PM | 219 | Panel Discussion: Advice and Mentorship from Female Leaders in Innovation and Entrepreneurship (Invited Talks)* | Orlando Ballroom N |
| Monday | 5:30 PM | 235 | MAC Eminent Engineers Awards Ceremony* | Regency Ballroom O |
| Tuesday | 8:00 AM | 244 | Advancing into Academic Leadership* | Plaza International Ballroom K |
| Tuesday | 8:00 AM | 261 | DORIC: Supporting Our Students with Disabilities | Bayhill 31 |
| Tuesday | 8:00 AM | 300 | Woman Chemical Engineers: Managing to Retain Them* | Bayhill 18 |
| Tuesday | 11:00 AM | 303 | MAC/MFF Real Talk: Navigating the Academic Career Path to Tenure (Ticketed Event)* | Gulf |
| Tuesday | 2:00 PM | 368 | The Current State of STEM Inclusion in the Workplace | Bayhill 23 |
| Tuesday | 3:30 PM | 412 | LGBTQ+ Inclusion in Engineering | Bayhill 23 |
| TD - Ammon | ia Energy | | | |
| Day | Time | Session # | Session Title | Room |
| Tuesday | 8:00 AM | 238 | Ammonia Synthesis: Intrinsically Carbon-Free Production | Regency Ballroom P |
| Tuesday | 10:20 AM | 302 | Ammonia Synthesis: Next Generation Technology I | Regency Ballroom P |
| Tuesday | 1:45 PM | 367 | Ammonia Combustion | Regency Ballroom P |
| Tuesday | 4:00 PM | 433 | Ammonia Cracking | Regency Ballroom P |
| Tuesday | 6:00 PM | 435 | Poster Session: Ammonia Energy | Regency Ballroom P |
| Wednesday | 8:00 AM | 436 | Ammonia Synthesis: Decarbonizing Hydrocarbon Feedstocks and Fuels | Regency Ballroom P |
| Wednesday | 10:20 AM | 494 | Ammonia Safety | Regency Ballroom P |
| Wednesday | 1:45 PM | 557 | Ammonia as a Fuel | Regency Ballroom P |
| Wednesday | 4:00 PM | 614 | Ammonia as an Energy Carrier | Regency Ballroom P |
| Wednesday | 6:00 PM | 616 | Ammonia Energy Association: Platinum Reception | Regency Ballroom P |

 $[\]ensuremath{^*}$ This session is co-sponsored by one or more programming groups

| Thursday | 8:00 AM | 617 | Ammonia Synthesis: Next Generation Technology II | Regency Ballroom P | |
|-------------------------------------|----------------|-----------|--|-----------------------------------|--|
| Thursday | 10:20 AM | 666 | Ammonia Synthesis: Next Generation Technology III | Regency Ballroom P | |
| Thursday | 1:30 PM | 715 | Ammonia Energy Implementation Conference: Plenary Session I | Regency Ballroom P | |
| Thursday | 3:30 PM | 749 | Ammonia Energy Implementation Conference: Plenary Session II | Regency Ballroom P | |
| TE - Advance | es in Fossil E | nergy R&D | | | |
| Day | Time | Session # | Session Title | Room | |
| Sunday | 3:30 PM | 10 | Advanced Materials for Carbon Dioxide Capture for Power Generation | Challenger 41/42 | |
| Sunday | 3:30 PM | 37 | Reaction Engineering for Combustion and Pyrolysis* | Plaza International Ballroom F | |
| Monday | 8:00 AM | 60 | Combustion Kinetics and Emissions* | Plaza International Ballroom F | |
| Monday | 8:00 AM | 90 | Novel Approaches to CO ₂ Utilization | Discovery 43 | |
| Monday | 12:30 PM | 127 | CO ₂ Use and Reuse | Challenger 41/42 | |
| Monday | 3:30 PM | 192 | Advanced Combustor Concepts | Challenger 40 | |
| Monday | 3:30 PM | 206 | Engineering Geologic Carbon Dioxide Storage Systems | Challenger 41/42 | |
| Tuesday | 8:00 AM | 253 | Breakthroughs in C1 to Chemicals and Processing Engineering* | Regency Ballroom Q | |
| Tuesday | 8:00 AM | 298 | Value-Added Chemicals from Natural Gas | Challenger 41/42 | |
| Tuesday | 12:30 PM | 308 | Advances in Methane Coupling Reaction and Aromatization | Challenger 41/42 | |
| Tuesday | 3:30 PM | 427 | Topical Plenary: Advances in Fossil Energy R&D (Invited Talks) | Challenger 41/42 | |
| Wednesday | 8:00 AM | 439 | Advances in Catalysis for Syngas Production | Challenger 41/42 | |
| Wednesday | 8:00 AM | 448 | Chemical Looping Processes* | Regency Ballroom Q | |
| Wednesday | 8:00 AM | 475 | New Technologies to Enhance the Production of Unconventional Oil & Natural Gas: Experimentation & Simulation | Challenger 40 | |
| Wednesday | 12:30 PM | 526 | Fuel Processing for Hydrogen Production | Challenger 41/42 | |
| Wednesday | 3:30 PM | 559 | Poster Session: Advances in Fossil Energy R&D | Regency Ballroom R/S | |
| Wednesday | 3:30 PM | 576 | Design and Optimization of Environmentally Sustainable Advanced Fossil Energy Systems | Challenger 41/42 | |
| Wednesday | 3:30 PM | 587 | Integrated Process Engineering and Economic Analysis* | Regency Ballroom Q | |
| Wednesday | 3:30 PM | 610 | Solid-Fluid Separations in Oil & Gas Production and Refining Processes* | Coral Spring I/II | |
| Thursday | 8:00 AM | 658 | Rare Earth Elements: Extraction, Separation, Characterization, Economics, Criticality, and Kinetics | Challenger 41/42 | |
| Thursday | 12:30 PM | 699 | Modular Processes for Coal and/or Biomass Conversion | Challenger 41/42 | |
| Friday | 8:00 AM | 752 | Applied Math for Energy and Environmental Applications* | Celebration 3 | |
| TF - Chemical Engineers in Medicine | | | | | |
| Day | Time | Session # | Session Title | Room | |
| Monday | 8:00 AM | 65 | Diagnostics, Treatments and Theranostics | Celebration 12/13 | |
| Monday | 12:30 PM | 122 | Chemical Engineers in Medicine Plenary I (Invited Talks) | Celebration 12/13 | |
| Monday | 3:30 PM | 222 | Precision Medicine, Big Data, and Chemical Engineering | Celebration 12/13 | |
| Tuesday | 8:00 AM | 277 | Medical Devices I | Celebration 12/13 | |
| Tuesday | 12:30 PM | 318 | Chemical Engineers in Medicine Plenary II (Invited Talks) | Celebration 12/13 | |
| Tuesday | 3:30 PM | 394 | Chemical Engineering Principles Advancing Medicine | Celebration 12/13 | |
| Wednesday | 8:00 AM | 467 | Medical Devices II | Celebration 12/13 | |
| Wednesday | 12:30 PM | 510 | Chemical Engineering Applications in Cancer | Celebration 12/13 | |

^{*} This session is co-sponsored by one or more programming groups

| TG - Innovati | TG - Innovations of Green Process Engineering for Sustainable Energy and Environment | | | | |
|---------------|--|-----------|--|----------------------|--|
| Day | Time | Session # | Session Title | Room | |
| Monday | 8:00 AM | 70 | Efficient Biological Processing of Lignin to Bioproducts and Biofuels | Regency Ballroom Q | |
| Monday | 12:30 PM | 134 | Efficient Chemical Processing of Lignin to Bioproducts and Biofuels | Regency Ballroom Q | |
| Monday | 12:30 PM | 165 | Career Paths: Perspectives by Minority Professionals in Chemical Engineering* | Regency Ballroom O | |
| Monday | 3:30 PM | 215 | Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Electrocatalyst Development | Regency Ballroom Q | |
| Tuesday | 8:00 AM | 253 | Breakthroughs in C1 to Chemicals and Processing Engineering | Regency Ballroom Q | |
| Tuesday | 12:30 PM | 345 | Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Material Innovations | Regency Ballroom Q | |
| Tuesday | 3:30 PM | 397 | Conversion of Solid Wastes to Energy and/or Product | Regency Ballroom Q | |
| Wednesday | 8:00 AM | 448 | Chemical Looping Processes | Regency Ballroom Q | |
| Wednesday | 12:30 PM | 555 | Topical Plenary: Frontiers in Green Process Engineering (Invited Talks) | Regency Ballroom Q | |
| Wednesday | 3:30 PM | 587 | Integrated Process Engineering and Economic Analysis | Regency Ballroom Q | |
| Thursday | 8:00 AM | 643 | Ionic Liquids: Properties and Thermodynamics | Regency Ballroom Q | |
| Thursday | 12:30 PM | 694 | Ionic Liquids: Novel Separation and Reaction Processes | Regency Ballroom Q | |
| TH - Synthet | ic & Renewa | ble Fuels | | | |
| Day | Time | Session # | Session Title | Room | |
| Monday | 8:00 AM | 103 | Synthetic Fuels Production from Natural Gas and Hydrogen | Regency Ballroom P | |
| Monday | 12:30 PM | 111 | Advances in Low-Cost Renewable Hydrogen Production at Large Scale | Regency Ballroom P | |
| Monday | 3:30 PM | 227 | Renewable Fuels Production from Captured CO_2 and Hydrogen | Regency Ballroom P | |
| TJ - Waste Pl | astics | | | | |
| Day | Time | Session # | Session Title | Room | |
| Sunday | 3:00 PM | 7 | Public Affairs and AIChE: A PAIC Town Hall* | Orlando Ballroom M | |
| Sunday | 3:30 PM | 34 | Polymers in Industry - Rising Stars (Invited Talks)* | Celebration 10 | |
| Monday | 12:30 PM | 166 | Sustainable Management and Uses of Post-Consumer Materials and Waste* | Regency Ballroom U | |
| Monday | 3:30 PM | 188 | Poster Session: Novel Products from Forest and Plant Biomass* | Regency Ballroom R/S | |
| Monday | 3:30 PM | 209 | Fundamentals of Sustainability Science and Engineering* | Blue Spring I/II | |
| Monday | 3:30 PM | 214 | In Honor of the 2018 R.H. Wilhelm Award Winner II (Invited Talks)* | Florida Ballroom B | |
| Tuesday | 12:30 PM | 332 | Fundamentals and Applications for Hazardous Waste Treatment* | Blue Spring I/II | |
| Tuesday | 3:30 PM | 395 | Climate Solutions* | Silver Spring I/II | |
| Tuesday | 3:30 PM | 405 | Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization* | Blue Spring I/II | |
| Wednesday | 12:30 PM | 555 | Topical Plenary: Frontiers in Green Process Engineering (Invited Talks)* | Regency Ballroom Q | |
| Wednesday | 3:30 PM | 560 | Poster Session: Catalysis and Reaction Engineering (CRE) Division* | Regency Ballroom R/S | |
| Wednesday | 3:30 PM | 574 | Composites for Energy and Environmental Applications* | Celebration 11 | |
| Thursday | 8:00 AM | 637 | Distributed Chemical and Energy Processes for Sustainability* | Regency Ballroom U | |
| Thursday | 8:00 AM | 661 | Sustainability and Consumer Products * | Regency Ballroom V | |
| Thursday | 12:30 PM | 691 | Going to a Decision Point in Sustainability Analysis* | Blue Spring I/II | |
| Thursday | 3:30 PM | 744 | Sustainability Metrics at the Process and Product Level* | Blue Spring I/II | |



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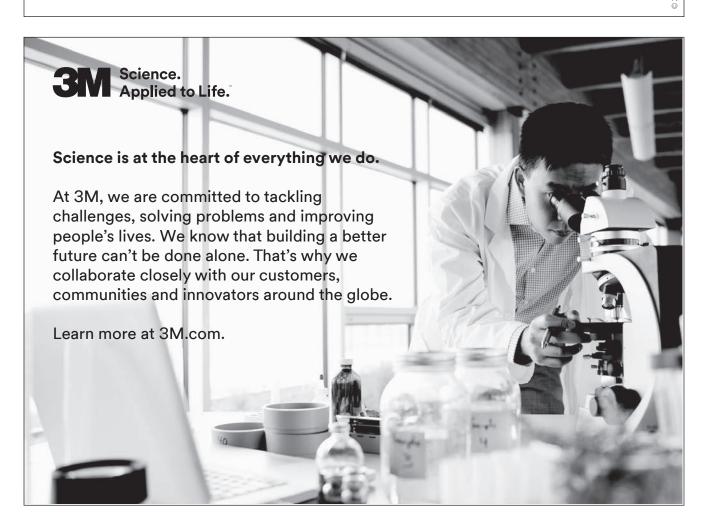
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MONDAY, NOVEMBER 11



TRANSFORMING THE ENGINEERING CLASSROOM WITH DIGITAL DATA TOOLSETS

9:15 AM - 10:30 AM | Hyatt Regency Orlando, Bayhill 24

Presenter: Chris Cogswell

In order to empower the engineering workforce to address the challenges they are solving, Elsevier has introduced several products to enable the understanding of complex engineering principles or content. 'Engineering Village' is a powerful search and discovery platform that provides data analytics tools for the analysis of engineering literature, including a numeric search tool which allows for searches of not just concepts but specific values of interest as well. 'Knovel' is a technical reference solution that provides answers and insights sourced from digitized and searchable engineering reference content, including critical reference titles and property databases. In this session we will introduce these tools and discuss how they can be used in the engineering classroom to better prepare for the transition to graduate school or the engineering workforce.



MAXIMIZE UPTIME WITH OPERATIONS ANALYSIS AND PRESCRIPTIVE MAINTENANCE

3:30 PM - 4:45 PM | Hyatt Regency Orlando, Bayhill 27

Presenter: Mike Brooks

There is a lot of talk these days about IIoT, Industrie 4.0, Digitalization, with Big Data, analytics, and machine learning. Not initiatives, these are technologies that support initiatives. In this session we'll explore how Operational Excellence is the real initiative, learn the supporting performance indicators, and explore maximizing uptime as the cornerstone of any attempt to improve operational excellence.

We'll take an in-depth look at examples of how prescriptive maintenance can provide early advance warning of failures, and guidance to identify the root causes of damage. With this knowledge, operations and maintenance staff can adjust conditions to eliminate the causes of most failures — acting with confidence to avoid process-related damage and consequent unplanned production downtimes. Or when a shutdown is unavoidable, at least plan the shortest, safest service and repair to mitigate the consequences.



ELECTROLYTE MODELING BASICS SIMULATION

3:30 PM - 6:00 PM | Hyatt Regency Orlando, Celebration 1 Presenters: James Berthold and Dr. Diana Miller

The Electrolyte Modeling Basics workshop is designed for attendees interested in learning about electrolyte chemistry concepts and the fundamentals of modeling electrolyte solutions. A lecture and hands-on OLI Studio and Flowsheet software exercises will be used to demonstrate how complex electrolyte systems can be modeled. Attendees will leave with a qualitative picture of how ions and molecules behave in water and a better understanding of solution properties such as alkalinity, pH, activity coefficients, and more. This course is appropriate for those new to OLI technology, professionals working with this software and those looking for a refresher course in its underlying theory. This course will provide a comprehensive overview of how electrolyte modeling can enhance process simulation results. Case studies such as refinery overhead corrosion simulation, RO membrane simulation for water treatment, and solvent extraction for metals and mining, among others, will be discussed.

TUESDAY, NOVEMBER 12



UTILIZING SEARCH TOOLS TO SPEED UP THE LITERATURE REVIEW PROCESS AND STAY AHEAD OF THE CURVE

9:15 AM - 10:30 AM | Hyatt Regency Orlando, Bayhill 33

Presenter: Chris Cogswell

Graduate research requires a broad knowledge of an underlying research field's literature, which can in many cases span decades of work. The effort going into these literature reviews can be significant at the front end of a graduate school career and can often make moving into new research areas or testing new applications for current research seem daunting for even experienced researchers. In order to help ease the understanding of the underlying research literature, as well as see how these areas connect to other research goals, Elsevier has a suite of tools which can be used to help make the literature more manageable and the underlying trends more apparent. In this session, we will discuss how to use these tools to promote overall understanding of the existing literature and find spaces where gaps exist, as well as improving knowledge of the underlying science required for valuable contribution in the lab. Specific topics will include utilizing faceted search strategies to begin a broad literature overview, numeric filtering for very detailed application searches, and generating search strategies to achieve the right results quickly using the tools 'Knovel' and 'Engineering Village'.



ASPEN KNOWLEDGE ACCELERATES BUSINESS INNOVATION

3:30 PM - 4:45 PM | Hyatt Regency Orlando, Rock Spring I/II

Presenter: Susmit Bapat

Innovation occurs when knowledge inspires the adoption of new technologies and work processes that drive improvements in yields and net production. In this session learn how our new offering, AspenTech Knowledge, provides the learning best practices that transform employee competence. Explore how AspenTech Knowledge accelerates adoption of new tools and technologies to improve operational excellence. Get ready for the future trends; see how implementing the AspenTech training certification program measures proficiency and assesses an engineer's potential for success. AspenTech offers many training programs that develop employee proficiency – customizable to unique company needs. Also, see how other companies use existing state grants to fund employee education.



HOW TO ACHIEVE PURITY, PRODUCTIVITY AND PROFITABILITY DEMANDS OF PROCESS INDUSTRY USING SIMULATED MOVING BED TECHNOLOGY

3:30 PM - 4:45 PM | Hyatt Regency Orlando, Celebration 1

Presenter: Trinath Pathapati

Complex streams in process industries require efficient downstream technologies. Simulated moving bed (SMB) chromatography has been known as a potential alternative to process multi-component streams. In the current workshop, we will focus on understanding the state of the art XPure SMB technology. This technology will then be assessed based on key industrial drivers like flexibility, operability and scalability. Finally, some tested and proven case studies will be presented. These cases will describe the impact of XPure SMB technology on purity, productivity and profitability requirements of specific industrial processes.

WEDNESDAY, NOVEMBER 13



CAPITAL ASSET LIFECYCLE MANAGEMENT (CALM) FOR CHEMICAL INDUSTRY

8:30 AM - 10:00 AM | Hyatt Regency Orlando, Bayhill 31

Presenter: Mallik Manem

CALM addresses the challenges of greenfield and brownfield capital projects, such as rampant delays and cost overruns, often caused by lack of system interoperability, low labor productivity and a failure to embrace digitalization. These challenges negatively impact the operational efficiencies of plants and facilities for decades. According to McKinsey & Company, 98% of megaprojects incur cost overruns or delays, averaging a cost increase of 80% and delaying delivery by 20 months. In addition, lack of accurate information results in operational inefficiencies through the life of the plant which is anywhere from 30-50 years. These numbers are staggering and provide a ripe opportunity for the application of Siemens solutions. In this session, you'll learn about the industry's major trends and challenges while conveying the power of digitalization and demonstrating its value throughout the lifecycle of plant or facility. You'll gain an understanding of Teamcenter for Capital Asset Lifecycle Management and how, through the dissemination of engineering and asset data, it can be used to spur your customer's digital transformation.



HOW TO DESIGN, BUILD AND IMPLEMENT INTEGRATED TECHNOLOGIES LIKE EXPANDED BED ADSORPTION IN SMB MODE

9:15 AM - 10:30 AM | Hyatt Regency Orlando, Celebration 11

Presenter: Trinath Pathapati

Bio-based industries need selective and efficient downstream solutions to process complex streams like fermentation broth. As fermentation streams contain both dissolved and suspended impurities along with large amount of water (> 70 wt%), it is required separate the impurities and also concentrate the product. In the current workshop, we will discuss the role of EBA technology as a smart separation step for bio-based streams and its impact on product purity, productivity and yield. We will then discuss the benefits of performing EBA in SMB mode and the approach to design, build and implement EBA-SMB. The design will focus on understanding the sensitivity of EBA and SMB technologies to different process parameters. The outcome of sensitivity analysis will then be used as design input for building a suitable and scalable hardware, software package for EBA-SMB integrated technology. Finally, a tested and proven case will be presented to describe the approach of implementing EBA-SMB and the resulting impact on process efficiency and economics.

WEDNESDAY, NOVEMBER 13 (CONTINUED)



THE PSE ACADEMIC TEACHING HIGHWAY (PATH) INITIATIVE - USING GPROMS FORMULATED PRODUCTS FOR DIGITAL **DESIGN OF PHARMACEUTICAL MANUFACTURING PROCESSES**

12:30 PM - 3:00 PM | Hyatt Regency Orlando, Bayhill 33

The PATH initiative aims to align the teaching of process modelling and related digital design techniques in universities with the needs of industrial employers, through the development and provision of software-agnostic teaching materials suitable for incorporation into undergraduate courses. This workshop will give a global overview on this initiative followed by a selection of a hands-on session on digital design of hydrogenation, crystallization and/or dry granulation using qPROMS FormulatedProducts. The workshop will provide an overview of how mechanistic modelling can be deployed to a number of pharmaceutical applications and will include the following elements:

- · Introudction to the PATH initiative
- Introduction to the unit operation modules within gPROMS FormulatedProducts
- Simulation of hydrogenation, crystallization and/or dry granulation processes (Hands-on)
 - Flowsheeting environment
- Manual scenario analysis of the impact of Critical Process Parameters (CPPs) on Critical Quality Attributes (CQAs)
- Introduction to Global System Analysis for conducting uncertainty & sensitivity analyses
 - Assessing the impact of CPPs on CQAs for each unit operation(Hands-on)

SIEMENS

SIMULATION FOR PERFORMANCE TWIN FOR PROCESS INDUSTRY

Ingenuity for Life 12:30 PM - 2:00 PM | Hyatt Regency Orlando, Bayhill 31

Presenter: Dr. Ravindra Aglave

Understanding of transport processes (fluid flow, heat transfer & mass transfer) is key for design, troubleshooting and exploring optimum operating conditions. 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 multi-physics simulation platform from Siemens. In this seminar we will look at successful deployment of such methods with industrial case studies.

We will also talk about how CFD & DEM simulation can be integrated in to process models/process simulation tools for a deeper insight. This portion will be presented by a quest speaker from Process System Enterprise (PSE)

All presenters will be available to answer questions.

SIEMENS

HOW TO SHAPE YOUR OWN AUTOMATION FUTURE WITH DIGITALIZATION

Ingenuity for life

2:30 PM - 5:30 PM | Hyatt Regency Orlando, Bayhill 31 Presenters: Jonas Norinder and Charlie Fialkowski

Digitalization is not a one-size, fits-all solution but rather a progression that varies greatly based on every company's systems, internal processes, and automation tools. To ensure that the right digitalization option is chosen at the right time, it is imperative to gain a holistic view of an operation by answering questions related to production needs, pain points, strategic goals as well as available time and investment. One way to ensure that all aspects of a digital transformation are considered, is to take a consultative approach that seeks to answer these questions with the aim of putting together a customized digitalization roadmap. This roadmap should go beyond standalone projects by assessing the latest developments in process control, analyzing the increasing amount of intelligence coming from smart field devices and review methods to capitalize on the information they provide. The intent is to first and foremost focus on implementing quick win projects with the most solid return on investment.

During this presentation you will gain the following insights:

- · A general understanding of key digitalization topics such as the digital twin, 3D, simulation as well as innovative ways of collecting data
- Learn about the importance of digital transformation
- Reasons to consider a consulting approach to create a customized roadmap
- What are latest developments in process control in the digital age
- How can information and data be used to more productively operate and maintain a plant?
- Why digital fieldbus technology is the most effective communication protocol in the digital age

THURSDAY, NOVEMBER 14



DIGITAL DESIGN OF ROBUST FORMULATED PRODUCTS

8:00 AM - 10:30 AM | Hyatt Regency Orlando, Celebration 8

Join PSE and industry experts for a hands-on software demonstration of gPROMS FormulatedProducts, an innovative and integrated platform for the digital design of robust formulated products and their manufacturing processes. The software enables a consistent methodology and workflow to be applied across the formulated products industries, using mechanistic models for process understanding, design space exploration, tech transfer, optimization, risk assessment, and product performance evaluation.

Scientists and engineers in the pharmaceutical, food, consumer goods, and specialty and agro-chemical industries will choose hands-on modules that demonstrate model configuration, validation with experimental data, optimization, and sensitivity analysis for a particular application. Modules include synthesis and fluid separation, crystallization, wet milling, filtration, continuous direct compression, wet and dry granulation, spray drying, oral absorption, and end-to-end flowsheet modelling.

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Highlights:

- Since its inception in 2007, ScaleUp has grown from 3,000 student members to over **24,000** to date.
- Since 2008, the AlChE's Safety and Chemical Engineering Education (SAChE) Certificate Program has awarded nearly **96,300+** certificates to students who have demonstrated proficiency in process safety training.

To learn more about a ScaleUp corporate sponsorship, visit www.aiche.org/scaleup or contact lan Sergo, Senior Director, Business Services, AIChE at ianse@aiche.org or 646.495.1518



INSTITUTE/BOARD AWARDS + MAJOR LECTURES

SUNDAY, NOVEMBER 10

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5:00 PM - 6:30 PM • Hyatt Regency Orlando, Plaza International Ballroom H Join your colleagues in honoring the recipients of the 2019 Board of Directors' and Institute Awards.

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FOUNDERS AWARD FOR OUTSTANDING CONTRIBUTIONS TO THE FIELD OF CHEMICAL **ENGINEERING**

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Elizabeth Sattely Associate Professor, Stanford University and The Howard Hughes Medical Institute



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Pablo G. Debenedetti Dean for Research, Princeton University



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(Award endowed by The AIChE Foundation)

Michael S. Strano Carbon P. Dubbs Professor of Chemical Engineering, Massachusetts Institute of Technology



AWARD FOR SERVICE TO SOCIETY

Gilda Barabino Dean and Daniel & Frances Berg Professor, The City College of New York



ENERGY AND SUSTAINABILITY AWARD

(Award sponsor: Air Products)

3M Cool Roofing Granules Team 3M Industrial Mineral Products Division



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Bindu Krishnan

Technical Leader, The Dow Chemical Company



INDUSTRIAL RESEARCH AND DEVELOPMENT AWARD

Mary T. am Ende
Vice President of Process
Development, Lyndra Therapeutics



INDUSTRY LEADERSHIP AWARD

Cristina U. Thomas
Senior Technical Leader and R&D Global
Process Owner, 3M



INSTITUTE AWARD FOR EXCELLENCE IN INDUSTRIAL GASES TECHNOLOGY Michael Baldea Associate Professor, University of Texas at Austin



LAWRENCE B. EVANS AWARD
IN CHEMICAL ENGINEERING PRACTICE
(The award is endowed by the AIChE Foundation)

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Paula T. Hammond Department Head; David H. Koch Professor, Massachusetts Institute of Technology.



IN CHEMICAL REACTION
ENGINEERING
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PRESIDENTIAL LECTURE

Monday, November 11 • 11:15 AM - 12:15 PM Hyatt Regency Orlando, Plaza International Ballroom H

The Valence of Skills: The Rise of Hybrid Jobs

Matt Sigelman, Chief Executive Officer, Burning Glass Technologies



D.I.C. WANG AWARD LECTURE

Monday, November 11 • 6:00 PM - 7:00 PM Hyatt Regency Orlando, Regency Ballroom V

From Artificial Cofactors to Synthetic Arrays: Teaching Old Enzymes New Tricks Douglas S. Clark, *Dean and G.N. Lewis Professor, University of California, Berkeley*



IACCHE'S JAMES Y. OLDSHUE LECTURE

Tuesday, November 12 • 8:00 AM - 10:30 AM Hyatt Regency Orlando, Plaza International Ballroom H

Response of Magnetic Nanoparticles to Time Varying Magnetic Fields: Ferrohydrodynamics, Nanoscale Thermal Therapy, and Magnetic Particle Imaging

Carlos Rinaldi, Chair and Professor, Department of Chemical Engineering and Professor, J. Crayton Pruitt Family Department of Biomedical Engineering, University of Florida



2019 ANDREAS ACRIVOS AWARD FOR PROFESSIONAL PROGRESS IN CHEMICAL ENGINEERING LECTURE

Tuesday, November 12 • 11:15 AM - 12:15 PM Hyatt Regency Orlando, Plaza International Ballroom H

Control of Interfacial Stability in Electrochemical Systems

Martin Z. Bazant, E. G. Roos (1944) Professor of Chemical Engineering and Mathematics and Executive Officer, Massachusetts Institute of Technology



SBE'S JAMES E. BAILEY AWARD LECTURE

Tuesday, November 12 • 6:00 PM - 7:00 PM Hyatt Regency Orlando, Regency Ballroom V

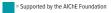
Systems Biology of Metabolism: Role in Production of Advanced Biofuels, Obesity and Cancer Jens B. Nielsen, *CEO, BioInnovation Institute* and *Professor, Chalmers University of Technology*



AWARD PRESENTATION

Biotechnology Progress Award for Excellence in Biological Engineering Publication

Michael L. Shuler, Samuel B. Eckert Professor of Chemical Engineering, Meinig School of Biomedical Engineering and Graduate Professor, Smith School of Chemical and Biomolecular Engineering Cornell University





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JOHN M. PRAUSNITZ AICHE INSTITUTE LECTURE Wednesday, November 13 • 11:15 AM - 12:15 PM

Hyatt Regency Orlando, Plaza International Ballroom H

From Chemical Engineering Fundamentals to the Commercialization of Vapor Deposited Polymers

Karen K. Gleason, Alexander and I. Michael Kasser Professor of Chemical Engineering, Massachusetts Institute of Technology



WILLIAM R. SCHOWALTER LECTURE

Wednesday, November 13 · 6:00 PM - 7:00 PM Hyatt Regency Orlando, Plaza International Ballroom H

Flowing Complex Fluids, from Blood to the Buffer Layer

Michael D. Graham, Vilas Distinguished Achievement Professor and Harvey D. Spangler Professor, University of Wisconsin-Madison

FEATURED SESSION

MEET THE INNOVATORS: TRANSFORMING THE FUTURE THROUGH CHEMICAL ENGINEERING

Tuesday, November 12 • 11:00 AM - 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom G

MODERATORS



Venkat R. Bethanabotla, Meeting Program Chair

Professor, Department of Chemical & Biomedical Engineering Director, Materials Science and Engineering Program, University of South Florida



Richard B. Dickinson, Meeting Program Co-Chair

Division Director, Chemical, Bioengineering, Environmental & Transport Systems Division, National Science Foundation, Professor, Department of Chemical Engineering, University of Florida

PANELISTS



CHEMICAL ENGINEERING INNOVATIONS FOR A RENEWABLE ECONOMY

Rakesh Agrawal

Winthrop E. Stone Distinguished Professor, Davidson School of Chemical Engineering, Purdue University



INNOVATIONS IN SYNTHETIC BIOLOGY

Jay D. Keasling

Professor, University of California, Berkeley and Senior Faculty Scientist, Lawrence Berkeley National Laboratory



ENGINEERING MATERIALS FOR CLINICAL APPLICATION

Christine E. Schmidt

Professor, J. Crayton Pruitt Family Chair & Department Chair, J. Crayton Pruitt Family Department of Biomedical Engineering, University of Florida







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The Minority Affairs Committee (MAC)

Celebrates the 2019 Eminent Chemical Engineers and the William W. Grimes Award Winner for Excellence in Chemical Engineering

Monday, November 11 5:30 PM - 7:00 PM Hyatt Regency, Orlando Ballroom O

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.



Dr. Emmanuel Dada* Assistant Professor *Prairie View A&M University*

* not presenting



Ms. Ana Davis Head, Health, Safety and Environment, North America Syngenta



Dr. Zenaida O. Gephardt Associate Professor *Rowan University*

William W. Grimes Award for Excellence in Chemical Engineering

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. Christine GrantProfessor and Associate Dean
North Carolina State University

Distinguished Service Award winner

MAC presents this award to recognize sustained service and outstanding achievements that advance the goals of the Minority Affairs Committee.



Dr. Belinda Akpa** Assistant Professor *North Carolina State University*

** Award presented at MAC reception



Promotes activities that will encourage the education and training of minorities in engineering and related disciplines.









Help Educate the Next Generation of Chemical Engineers in Process Safety

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A global initiative that is defining how the next generation of chemical engineers are prepared to enter the workforce. A core priority of our 'Doing a World of Good' campaign, the program incorporates process safety training into the chemical engineering curricula at universities throughout the world in order to ensure that every chemical engineering graduate has a working knowledge of process safety.

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2019 TECHNICAL PROGRAM GRID

(1) Undergraduate Professional **Workshop for Women & Minorities** - hosted by Women in Chemical **Engineering (Ticketed Event)** Sunday, Nov 10, 9:00 AM

Hyatt Regency Orlando, Barrel Spring I

Sponsored by: Women in Chemical **Engineering Committee (WIC)**

(2) Women in Chemical Engineering (WIC) presents "Elevating Your Career for Graduate Students and Young Professionals" (Ticketed Event)

Sunday, Nov 10, 9:00 AM Hyatt Regency Orlando, Barrel Spring II

Sponsored by: Women in Chemical **Engineering Committee (WIC)**

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

Sunday, Nov 10, 4:15 PM Hyatt Regency Orlando, Orlando Ballroom M

Sponsored by: Young Professionals Committee (YPC)

4:15 Introductory Remarks

4:18 YCOSST Award Presentation to Prof. Kory C Russel for University of Oregon project on "Sanitary Green Space: a Closed-Looped Sanitation System for Growing Green Communities"

4:30 Paper 3a: Preparing for the Worst: The Case for Solar Geoengineering Research and Oversight

- Bradie S Crandall

4:45 Paper 3b: Addressing Management Challenges Within the Nuclear Weapons Complex to Streamline Plutonium Disposition

- Cameron Hong

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

Sunday, Nov 10, 10:00 AM Hyatt Regency Orlando, Rock Spring I/II **Timothy Anderson, Chair**

Sponsored by: Career Guidance **Committee Liaison**

(5) Chem-E-Car Competition Sunday, Nov 10, 12:30 PM

Hyatt Regency Orlando, Windermere **Ballroom**

Sponsored by: Student Chapters Committee Liaison

(6) Meet the Faculty and Post-Doc Candidates Poster Session

Sunday, Nov 10, 1:00 PM Hyatt Regency Orlando, Regency Ballroom R/S

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

Sponsored by: Meet the Faculty and Post-Doc Candidates Poster Session --Sponsored by the Education Division

■ BIOMATERIALS & BIOLOGICAL ENGINEERING

Paper 6b: Engineering the Future of Aging, Healthspan and Lymphoma Time Jude M. Phillip

Paper 6d: Designer Biomaterials and Integrated Biosensors Toward Precision Medicine

- Jouha Min, Ralph Weissleder

Paper 6e: Biomaterial Investigation and Development for Biomedical Advancement

- Antonio C. F. dos Santos

Paper 6f: Molecular Simulations of **Biological Self-Assembly**

Gul H. Zerze

Paper 6h: Peptide- and Protein-Based Functional Biomaterials

- Jugal Kishore Sahoo

Paper 6i: Conversion of Waste Biomass into Bioproducts (Bioenergy, Biomaterials, Biochemicals)

Ezinne Achinivu

Paper 6k: Engineering Biology Solutions for a Sustainable Future

- Niju Narayanan

Paper 6n: Exploring the Design Space of Living Systems: Experimental and Theoretical Tool-Kits for Multi-Functional Materials

- Symone Alexander

Paper 6r: Ultrasmall C' Dots Activate Pro-Inflammatory Anti-Tumor Responses in the Microenvironment of PDGF-B Driven High Grade Gliomas

- Steven Zanganeh

Paper 6s: Metabolic Sugar Labeling for Cancer Targeting and Immunoengineering

- Hua Wang, David J. Mooney

Paper 6u: Multiscale Dynamics in Biological Soft Matter and Polymeric Fluids

Amir Saadat

Paper 6v: Molecular Tension Sensors in Protein Hydrogels

— Joshua Baccile, David Tirrell

Paper 6w: 3D-Engineering of Functional Living Composite Materials

- Seunghyun Sim

Paper 6z: Regenerative Bandages for Enhanced Healing in Diabetic Wounds

Sahar Rahmani

Paper 6ab: Molecular Design Principles for Chemically Tunable Biomaterial Platform Technologies

— Crystal K. Chu

Paper 6ac: Shining Light on the Nervous System: From Biomaterials to **Bioelectronics**

Jing Tang

Paper 6ae: 3D Printed Bioelectronics for Tissue Engineering and Regenerative Medicine

Alexandra Rutz

Paper 6ag: Lipid Nanoparticles for Highly Efficient Non-Viral Gene Editing Jie Li, Niren Murthy

Paper 6iz: Multiscale Modeling for the **Design of Functional Soft Materials** — Nicholas Jackson

Paper 6g: Fabrication of Highly Sensitive LSPR Biosensor for the C-Reactive Protein (CRP) Detection Based on the Immunocolloidal Gold Nanoparticles

- Seo Yeong Oh, Tea-Joon Jeon, Eunseon Lee, Mi-Wha Oh, Yun Suk Huh

Paper 6y: Multiscale Biomechanics of Platelet-Driven Blood Clot Contraction and Intracellular Mechanisms of Its Termination

— Oleg Kim

Paper 6kk: Hierarchical Self-Assembly and Biological Interactions of Functional Synthetic and Natural Supramolecular Systems

— Herdeline Ann M. Ardoña

Paper 6kq: Genetically Engineered Probiotics Designed at the Interconnect of Synthetic Biology and Metabolic Engineering

- Amin Zaraar

Paper 6kr: Quantitative Single-Cell Analysis of RNA Regulation at the Single Molecule Level

– Fangyuan Ding

Paper 6ks: Theory and Modeling of Biopolymers and Bio-Inspired Soft Materials

– Kai Huana

Paper 61: Understanding Physically Crosslinked Polymer Networks to Rationally Design Hydrogel Biomaterials — Hector Lopez Hernandez, Eric A.

Paper 6m: Biocompatible Zwitterionic Polymers for Medical Applications

- Xiaojie Lin

Paper 6p: Electrochemistry Enabling New Frontiers in Biomaterials Engineering

– Sina Jamali

Paper 6t: Tailoring Polymer Chemistry for Biomass-Derived Materials: From Artificial Plant Cell Wall to Fungible **Bioproducts**

— **Qiang Li**, Joshua Yuan

Paper 6x: Interactive Characterization of Biomaterials in Simulated Biological Environment

— Sina Jamali

Paper 6ah: All-Atom Molecular Dynamics Simulations of the 5-HT₂B G Protein-Coupled Receptor

- Brandon Peters, Andrew Ferguson

Paper 6aa: Engineering Microorganisms and Their Environment for Increased Performance in Biorenewable Applications

- Kirsten Davis

Paper 6a: Nano-Optical and -Electronic Devices with Machine Learning for Biomarker Discovery and Diagnostics in Personalized Medicine

— Lee Korshoi

Paper 6c: Biosafe, Eco-Friendly Levan Polysaccharide Toward Transient Electronics

- Kiyoon Kwon, Tae-il Kim

Paper 6j: Constitutive Modeling of Complex Biomaterials

Jeffrey S. Horner

Paper 6o: Integrating Molecular Modeling with Experimental Work to Propel a Bioproducts Pipeline

- Emma C. Brace

Paper 6af: Advancing Technologies for Prenatal and Women's Health

- Christina M. Bailey-Hytholt

Paper 210a: Biofilm Prevention By UVC Side Emitting Optical Fibers

- Mariana Lanzarini-Lopes, Sergi Garcia-Segura, Paul Westerhoff

Paper 6kt: Force Response Defines Both Subcellular Architectures and Dynamic Protein Binding

- Peter Chung

Paper 6kw: Engineering Biomimetic Materials and Cells for Diagnostic and Therapeutic Applications

– Zongmin Zhao

Paper 6kz: Multi-Modal Biofabrication Approaches for Biomaterials **Development and Tissue Engineering**

— Jenna M. Shapiro

Paper 6le: An Unsteady State Reactor **Engineering Model for Spatially** Heterogeneous Wine Fermentations - Konrad Miller, David E. Block

BIOMEDICAL ENGINEERING

Paper 6ai: Living Biodevices for Precision Medicine:from Morphing Electronics to Medical Nanorobots

— Jinxing Li

Paper 6aj: Soft, Flexible Tissue-Integrated Chemical Sensors: From Wearable to Implantable Neural Systems — Amay J. Bandodkar, John A. Rogers Paper 6ak: Lung Surfactant Inhibitors and Their Effect on ARDS (Acute Respiratory Distress Syndrome)

— Sourav Barman

Paper 6al: Developing Tools for Emerging Liquid Biopsy Applications

— Jose C. Contreras-Naranjo

Paper 6am: Interfacing Cell/Tissue Engineering with Gene Editing Tools and Sequencing Technologies for Regenerative Medicine

— Halil Tekin

Paper 6an: Engineering Microsystems for Regulating Cellular Behavior: From Implantable Drug Factories to Novel Platforms for Single-Cell Genomics

— Suman Bose

Paper 6ao: Biologically Inspired, Electrically Active Membranes for Sustainability and Medicine

- Thomas B. H. Schroeder

Paper 6ap: Computational Modeling in Cancer Systems Biology: Stochasticity, Complexity, and Multiscale Dynamics in Disease Progression and Drug Response

— Leonard Alfredo Harris

Paper 6aq: Engineering the Tumor Microenvironment

— Andreas Kourouklis

Paper 6ar: Multidimensional Single Cell Analysis: Devices and Technology for Cancer Biology

— Alex Xu

Paper 6at: The Role of Topographical Cues in Cancer Cell Migration and Metastasis

— Colin D. Paul

Paper Gau: Reverse Perfluorocarbon Emulsions for Pulmonary Drug Delivery

— Diane L. Nelson

Paper Gav: Engineering DNA-Polymer Assemblies

— Alexander E. Marras

Paper 6aw: Synergizing Engineering, Chemical, and Immunological Concepts to Design the Next Generation of Therapeutics for Unmet Clinical Needs

— Benjamin Umlauf

Paper 6ax: Engineering Materials to Recapitulate the Stem Cell Microenvironment

- Christopher M. Madl

Paper 6ay: Ionic Liquids to Overcome Obstacles in Nanoparticle Drug Delivery

— Eden E L Tanner

Paper 6ba: Understanding Nucleation and Crystal Growth of Organic Molecular Materials with Application to Pharmaceutical Manufacturing

— Gerard Capellades

Paper Gas: A Polymeric Reactor for the Synthesis of Superparamagnetic-Thermal Treatment of Breast Cancer

— Roa' Fardous

Paper 6ka: Membrane Remodelling by Proteins and Self-Assembled Nanostructure

— Amir H. Bahrami, Carol Hall

CATALYSIS

Paper 6bc: Process Intensification for Sustainable Fuels and Energy Production

— Cornelius Mduduzi Masuku

Paper 6bd: Molecular Modeling and Machine Learning for Catalysis and Separations

- Tyler R. Josephson

Paper 6be: Developing Active, Selective, and Energy-Efficient Heterogeneous Catalytic Processes for Enhanced Sustainability

- Insoo Ro

Paper 6bg: Scaling up First Principle Simulation in Realistic Environment: Solvent Effects and Excited State Properties in Computational Catalysis — Fang Liu

Paper 6bh: Elucidating Atomic Dances through Reaction Landscapes

- Arthur J. Shih

Paper 6bi: From 1- and 2-Dimensional Materials to Architectural Properties in Catalysis: Rationalizing, Predicting and Designing through First-Principles Methods

- Roberto Schimmenti

Paper 6bk: Dynamic Heterogeneous Catalysis to Enhance Turnover Frequency Via Surface Resonance

- M. Alexander Ardagh

Paper 6bl: Development of Next-Generation Catalytic Technology for Efficient and Sustainable Chemical Transformations

- Manish Shetty

Paper 6bm: Sustainable Fuel and Chemical Synthesis Via Catalytic Valorization of Abundant and Renewable Resources

- Nathaniel Eagan

Paper 6bn: Discovery and Optimization of Processes and Catalysts for the Organic Electrosynthesis of Carbon-Neutral Fuels and Chemicals

— Ezra L. Clark

Paper 6bp: Enabling New Chemistries through Catalyst Design

- Marcella Lusardi, Mark E. Davis

Paper 6bq: Precision Synthesis to Control Catalyst Surface Structures for Improved Reactivity and Performance

— Madelvn R. Ball

Paper 6bs: Reshaping the Carbon Cycle with Catalysis: Selective Activation of Chemical Bonds for Producing Carbon Neutral Fuel and Chemicals

Alyssa Hensley

Paper 6bu: Development of Thin Film Deposition & Etching Processes for Challenging Materials

— David Barlaz

Paper 6bv: Unifying Principles in Thermally and Electrochemically Driven Catalytic Reactions

— Joaquin Resasco

Paper 6bz: Fixed Feed Temperature Program Modulation (FFTPM) - a Versatile Method for Extracting Adsorption Thermodynamics for Weakly Adsorbing Systems over a Range of Adsorbates

- William T. Gibbons

Paper 6ca: Mechanistic Study and Engineering of Vapor/Solid Interface in-Operando: Applications in Heterogeneous Catalysis for Energy Upgrading Reactions

- Xuegiang Zhang

Paper 6cf: Understanding and Controlling Multielectron Transfer Chemistry for Sustainable Energy Technologies

- Adam Nielander

Paper 6ch: Computational-Accelerated Materials Design for Negative Emission Technologies

- Paul Meza-Morales

Paper 6ci: Catalyst Design through Simulations and Machine Learning

- Seoin Back

Paper 6cj: Accelerating Net-Zero Carbon Emissions By Electrochemical Catalysis: Understanding and Controlling the Reactions at Interfaces

— Lei Wang

Paper 6kg: Design of Dynamic and Solvated Reaction Environments for Enhanced Conversion and Selectivity with Heterogenous Catalysts

— Jennifer Jocz

Paper 6kn: Sustainability towards the Future:bridging the gap between catalysis science and reaction engineering

— Yang Xiao

Paper 6bx: Bimetallic Catalysts for Internal Steam Reforming of Methane at Low-Temperature for High Fuel Utilization of Proton-Conducting Ceramic Fuel Cells

— Kvunapvo Hona

Paper 6cd: Rational Catalysts and Process Development for Light Hydrocarbons Upgrading from Natural Gas/Shale Gas

— Weijian Diao

Paper 6bb: Rational Design of Alloy Catalysts By Building Atomic-Scale Structure-Property-Activity Relationships

— Liang Cao

Paper 6bj: Combining First-Principles Modeling and Nanomaterial Synthesis to Understand and Improve Environmental Catalysis

— Hanvu Ma

Paper 6ck: Process-Informed Design of Electrocatalysts for Sustainable Chemical Transformations

– Gastón O. Larrazábal

Paper 6cg: Development of n-Doped Oxides As an Electron Rich Support: Bridging Homogeneous and Heterogeneous Catalysis

— Juan Jimenez

Paper 6bf: Fundamental Design of Sustainable Catalytic Reactions at the Water-Energy-Food Nexus

— Lea Winter

Paper 6bo: Electrosynthesis for Sustainable Chemical Production

- Matthew Jouny

- Gabriel Seufitelli

Paper 6br: Study of Catalytic Reactions for the Production of Fuels and Chemicals from Renewable Feedstocks

Paper 6bt: Direct and Non-Oxidative Conversion of Methane to Value Added Products

- Vaidheeshwar Ramasubramanian

Paper 6bw: One-Step Synthesis of Oxide Catalysts Using Aerosol Reactors for Environmental Applications: Theoretical and Experimental Study

— Sungyoon Jung

Paper 6cb: Engineering the Catalytic Environment: Synthetic, Mechanistic, and Spectroscopic Approaches for Developing Design Principles

- Daniel T. Bregante

Paper 6cc: First-Principles Approaches for Catalyst Design: Novel Descriptors and Strategies for Materials Discovery

— Joseph Gauthier

Paper 6ce: Study on Fe-Mo/CAR Bifunctional Catalyst for One-Step Synthesis of Methylal Via Methanol Oxidation

— **Meng Yuan**, Yuanyu Tian, Qiao Yingyun

Paper 6ku: Novel Approaches to Biomass Upgrading for a More Sustainable Chemical Industry

- Andrew W. Tricker

Paper Glc: Catalyst Design with Atomic Precision for Fuel Gas Processing and Pollution Purification Reactions — *Ming Yang*

■ COMPUTATION & MODELING

Paper 6cl: Molecular Simulations of Interfacial Dynamics in Biological Systems — *Viviana Monje-Galvan*

Paper 6co: Reproduce - Remediation and Production Using Computational and Electrochemical Approaches

— Damilola A. Daramola

Paper 6cx: Diffusion in Biophysics, from Protons to Cargo: A Model System Approach

— Steven Strong

Paper 6cz: From Biosynthesis to Human Health: Harnessing Biomolecules with Multiscale Quantum Mechanics— Molecular Mechanics Simulations

- Zhongyue Yang, Heather J. Kulik

Paper 6jx: Designing the Structure and Function of Soft, Complex Materials with Computational Modeling

— Michael P. Howard

Paper 6ki: Computational Protein Design Using Optimization Programs and Force-Field Calculations

— **Ratul Chowdhury**, Costas Maranas, Manish Kumar **Paper 6cp:** Data-Driven Modeling and Control of Batch and Batch-like Processes

— Abhinav Garg

Paper 6cq: Optimization and Control of Chemical Process Systems Under Uncertainty

— Rohit Kannan

Paper 6cr: Computational Design and Development of Advanced Catalytic Materials

- Mingjie Liu

Paper 6cs: Studying Soft Materials inand out-of-Equilibrium Using Analytical and Numerical Field Theories

- Douglas Grzetic

Paper 6ct: QM-Based Multiscale Simulations for Applications in Electrocatalysis, Interfacial Chemistry, and Energetic Materials

- Saber Naserifar

Paper 6cu: Computational Heterogeneous Catalysis for Energy Storage and Conversion

— Zhenghang Zhao

Paper 6cv: Computational Crystallization and Assembly of Polymers and Soft Matter

— Wenlin Zhang

Paper 6cw: Computational Modeling of Chemical Interactions at Interfaces for Environmental Applications

- Zhizhang Shen

Paper 6cy: Modeling and Optimization for Process System Engineering Problems

— Yachao Dong

Paper 6da: Combining Computational Chemistry and Advanced Characterization for Process Optimization and Intensification

— Adam Karcz

Paper 6db: Predictive Descriptors for the Targeted Synthesis of Solid-State Materials

- Christopher J. Bartel

Paper 6cn: Understanding Multimodal Interactions through Deep Neural Networks and Statistical Mechanics

— Camille Bilodeau

EDUCATION

Paper 6dc: Investigating Biophysical Interactions Using Coarse-Grained Simulations

— Katelyn Dahlke

■ ELECTROCHEMISTRY

Paper 6dd: Mechanistic
Electrochemistry Driving Energy
Science: From Catalysts to Batteries
— Srini Ramakrishnan, Byungchun
Park, Robert M. Waymouth, Christopher
E. D. Chidsey, Bryan D. McCloskey

Paper 6di: Heterogeneous Electrocatalysis: Developing Strategies to Engineer Industrially Relevant Catalysts from Fundamental Activity Trends

— Michaela Burke Stevens

Paper 6dj: From Molecular-Level Catalyst Design to Reactor-Level Integration for Energy Conversion Technologies

- Molly Jhong

Paper 6dm: Chemically and Electrochemically Interactive Characterization of Biomaterials in Vitro — Sing Jamali

Paper 6dn: Corrosion Mitigation and Wastewater Treatment

Zineb Belarbi

Paper 6do: Nanoscale Design of Electrocatalysts for CO₂-to-Fuels Powered Using Renewable Electricity

- Yuguang (Chris) Li

Paper 6dp: Reinforced Anion Exchange Membrane (AEM) Separators Based on Triblock Copolymers for Electrode-Decoupled Redox Flow Batteries (RFBs)

— Shrihari Sankarasubramanian

Paper 6df: Developing Electrochemical-Based Predictive Battery Health Monitoring for Future Battery Management Systems

— Saeed Khaleghi Rahimian

Paper 6de: Charge Storage and Transport in Electrochemical Science: From Bulk to Interfaces

— Chia-Chin Chen

Paper 6dg: Electrocatalysts and Gas Diffusion Electrodes for Vapor-Phase Carbon Dioxide Electrolyzers and Hydrogen Fuel Cells

— **Dong Un (Daniel) Lee**, David Koshy, Kabir Abiose, Daniel Corral, Christopher Hahn, Thomas F. Jaramillo

Paper 6dh: Combining Advanced Materials and Manufacturing and Electrochemical Engineering for Building a Sustainable Future

— Jeremy T. Feaster

Paper 6jy: Design of Electrochemical Biosensing Strategies Toward High-Sensitivity, Non-Fouling, Multiplex Point-of-Care Systems

— **Yifan Dai**, Xiaowei Wu, Jiwei Yao, Yinuo Chen, Yuan Wang, Wei Xu, Le Luo, Liang-yuan Chiu, Jianzhi Huang, Huichun Zhang, Blanton Tolbert, Chung-Chiun Liu

■ ENERGY & SUSTAINABILITY

Paper 6dq: Advanced Materials for Efficient Energy Conversion Based on Spectroscopic and Mechanistic Study

— **Xuan Yang**, Yushan Yan, Bingjun Xu

Paper 6dx: Fabrication of Conducting Polymers and Superconductors Using Chemical Vapor Deposition Methods for Energy and Electronic Application

— Meysam Heydari Gharahcheshmeh

Paper 6dy: Sustainability in Process Systems Engineering

— Styliani Avraamidou

Paper 6dz: Oxygen Reduction Reaction (ORR) and Oxygen Evolution Reaction (OER) Bifunctional Electrocatalyst Fabrication for Unitized Regenerative Fuel Cell (URFC) Application

— Pralay Gayen

Paper 6ea: Nanostructured Materials for Next-Generation Lithium-Sulfur Batteries

- Somayeh Zamani, Yong Lak Joo

Paper Geb: Kinetics and Chemistry of Fast Pyrolysis of Carbon-Based Material Using Novels Reactors Approaches

- Ali Zolghadr

Paper 6ec: Energy Storage and Conversion with Organic Molecules and Advanced Porous Electrodes

- Michael R. Gerhardt

Paper 6ed: Materials for Energy Storage Applications: Fundamental Insight for Rational Design and Development

- Jeffrey Lopez

Paper 6eh: Realizing CO₂ Utilization and Carbon-Neutral Energy Conversion in Practical Scenarios --- Mining the Air, Extracting Industrial Wastes, One-Pass Conversion, and Scale-Out

— Xu Li

Paper 6ei: Advancing the Development of Fuel Flexible Combustion, Compact Energy Systems, and the Sustainability Analysis Methods

- Sampath Gunukula

Paper 6en: Electrochemical Engineering for Energy, Environment and Separation Applications

— Tao Gao

Paper 6kj: Illuminating Solid-Water Interfacial Processes at Nanoscale for Sustainable Environmental Remediation and Resource Recovery

— Haesung Jung

Paper 6dr: Winning the Energy Dilemma: Carbon-Free Energy and Environmental Sustainability

— Simona Liguori

Paper 6du: Organic Molecular Electrocatalysts for Energy-Water Nexus and Beyond

— Xi Yin

Paper 6ej: Energy Conversion and Storage

— Yijin Kang

Paper 6ek: Efficient Carbon Modification for Sustainable Food/ Energy/Water Nexus

— **Baharak Sajjadi**, Wei Yin Chen, Daniell Mattern

Paper 6eo: Multiscale Approach to
Future Energy Science and Engineering
— Yingda Lu

Paper 6el: Biopolymer Encapsulated Lipase for Biodiesel Production

— Ravindra Pogaku

Paper 6kp: Functionalized Materials for Sustainable Energy Applications: Structure and Reactivity

— Gengnan Li

Paper 6dt: Sustainable Conversion Processes and Reactor Design to Produce Fuels and Chemicals

- Muhammad Siddiquee

Paper 6ee: Sustainable Energy Production from Renewable and Fossil Fuels

- Saikat Das

Paper 6ef: A Structured Approach to the Design and Optimization of Sustainable Energy Systems

- Nathanial J. Cooper

Paper 6em: The Future of Concentrated Solar Thermal - Smart Selection of Materials for Hydrogen Production and Energy Storage

- Alicia Bayon

Paper 6ke: Moving Beyond the Limits between Science, Engineering and Information Technology for a Sustainable Society and Economy

— Botond Szilagyi

Paper 6ds: A Novel Route for the Flexible Preparation of Hydrocarbon Jet Fuels and Valuable Chemicals from Biomass-Based Platform Chemicals: A Case of Using 2, 3-Butanediol As a Feedstock

— **Yuchen BAI**, Xuebing Zhao, Dehua Liu

Paper 6If: Engineering Multifunctional Nanomaterials for Energy and the Environment

- Michael Bozlar

FLUID MECHANICS

Paper 6ep: Active Soft Materials: Data Driven Study to Understand, Control, and Design Bio-Soft-Materials

— Mehdi Molaei

Paper 6eq: Dynamics, Transport, and Self-Assembly in Flowing Polymeric Liquids

— Sarit Dutta

Paper 6et: Constitutive Modelling for Complex Fluids in Complex Flows

— Joseph Peterson

Paper 6ev: Structure, Rheology and Processing of Complex Fluids Towards Scalable Manufacturing of Functional Devices

- Sunilkumar Khandavalli

Paper 6ew: Complex and Biological

— Debasish Das

Paper 6kl: Microscale Transport Phenomena: Data Analytics and Fluid Dynamics

- Shiyan Wang

Paper Geu: Mathematical Modelling and Computational Fluid Dynamics Analysis of Lamp Amplification Reaction on a Porous Paper Membrane - Point of Care Diagnostic Prespective

— Debayan Das

Paper Ger: Leveraging Soft Matter Flows across Length Scales to Improve Human Health

— Aditya Raghunandan

Paper 6es: Dynamics of Soft Material Systems Under Electric Fields — Rajarshi Sengupta Paper 6kx: Investigating Yielding Dynamics and Fracture Mechanics in Soft Materials

- Alan Ranjit Jacob

■ INTERFACIAL & TRANSPORT PHENOMENA

Paper Gex: Understanding and Designing Non-Equilibrium States at Soft/Hard Material Interfaces

— Yanhao Yu

Paper Gey: Quantifying Interfacial Transport Phenomena for Environmental and Biochemical Systems

- Henry C. W. Chu

Paper Gez: Microbial Biofilm Processes: Multiscale Modeling, Simulation, and Visualization

— George E. Kapellos

Paper 6fb: Design of Functional Soft Materials for a Sustainable Future

— Karthik Nayani

Paper 6fd: Intelligent Systems, Active Colloids, and Advanced Responsive Materials

— Nicholas G. Chisholm

Paper 6ff: Designer Soft Matter: From Passive to Active to Biomimetics

— Hanumantha Rao Vutukuri

Paper 6fg: Coupled Ion Transport and Fluid Flow in Energy and Environmental Sciences

- Mohammad Mirzadeh

Paper 6fh: Dilational Rheology of Lung Surfactant Inhibitors and Its Effects on Acute Respiratory Distress Syndrome — Souray Barman

Paper 6fi: Ionic and Electronic Transport Properties in Covalent Organic Framework and Nanomaterial

— Ankit Agrawal

Paper 6fa: From Understanding the Transport of Complex Fluids to Development of Liquid Lenses — Shreyash Gulati

Paper 6fe: Flow of Soft Matter in Complex Geometries

— Yu-Jiun Lin

Paper 6fc: Role of Species Transport on the Stability of Interfaces

- Vineeth Chandran Suja

MATERIALS

Paper 6fk: Silk-Based Materials: A Sustainable Route Towards Multifunctional Material Applications

— Jaewon Choi

Paper 6fm: Interfacial Materials for Electrochemical and Biomedical Devices — Jie Zhao, Yi Cui, John A. Rogers

Paper 6fn: Machine Learning and Data-Enabled Design and Discovery of Soft and Nano Materials

— Tarak Patra

Paper 6fq: Rational Design of Smart Soft Materials

— Yimin Luo

Paper 6fr: Tailoring Organic Materials for Electronics and Energy: From Molecular Design to Two-Dimensional Polymerization

— Yu Zhong

Paper 6fs: Learning from Nature: Rational Design of Multifunctional Hybrid Materials

- Hyosung An

Paper 6fu: Rational Design of Advanced Materials and Membranes for Energy, Separations and Catalytic Applications

- Sameh Elsaidi

Paper 6fx: Highly Energy-Dense, Rechargeable, Alkaline Birnessite-Zinc Batteries for Grid-Scale Applications

- Gautam G. Yadav

Paper 6fp: Understanding the Synthesis Pathways of Inorganic Functional Materials

- Bor-Rong Chen

Paper 6ft: Computational Assembly Engineering for Bio-Inspired Nanomaterials

- Trung Nguyen

Paper 6kd: Hierarchically Engineered Structures Using Self- and Directed-Assembly for Unique Electronic, Optical and Mechanical Properties

— Yuyin Xi

Paper 6fj: 3D Printing of Polylactic Acid Mixed with Wood

- Samarthya Bhagia

Paper 6fv: Advance Manufacturing of Materials for Flexible and Stretchable Devices

- Kunal Mondal

Paper 6fw: Bio-Inspired Soft Electronics

— Alex Chortos

Paper 6fo: Scalable Synthesis of Nanoand Micro-Scale Materials for Energy Applications

— Clayton Kacica

Paper 6kc: Molecular Engineering Approach for the Development of Advanced Functional Materials: Engaging Students Through Impactful Research

— Anthony Engler

Paper 6lb: Polymer Science in Developing Fibrous materials for Advanced Technical Applications

— Behzad Nazari

NANOMATERIALS & NANOTECHNOLOGY

Paper 6fz: Advancing Nanomaterials for Energy and Water Applications Using Atomistic and Quantum Chemical Simulations

— **Ananth Govind Rajan**, Michael Strano, Daniel Blankschtein, Emily A. Carter

Paper 6ga: Catalytic Porous Materials with Tailored Nanostructures for Selective and Sustainable Chemical Processes

— Hong Je Cho

Paper 6gb: Building Autonomous Nanomachines at the Interface of Colloids and Electronics

— Volodymyr Koman

Paper 6gd: Controlling Organization and Effects of Nanoparticles on Polymer-Nanoparticle Composites

— **Hamed Emamy**, Oleg Gang, Francis W. Starr, Sanat K. Kumar

Paper 6ge: Engineering Redox-Active Materials from Electrocatalysis to Pseudocapacitance

- Xueli Zheng

Paper 6gf: Engineering Nanomaterials for Biomedical Applications

- Devleena Samanta

Paper 6gi: An Active Approach to Colloidal Self-Assembly

- Stewart Mallory

Paper 6gj: Low-Cost, Scalable, and Rapid Platforms in Ultrathin Materials Synthesis for Water and Energy Technologies

- David S. Bergsman

Paper 6gn: Nanostructured Anodic Oxides of Metals: From Corrosion Protection to Nanotechnology and Emerging Applications

— **Wojciech Stepniowski**, Wojciech Misiolek, Kuo-Kuang Wang

Paper 6go: Electrochemical and Optoelectronic Transformations in Dynamic Semiconductor Nanomaterials

— Clayton J. Dahlman

Paper 6gp: Applications of Nanofillers in Advanced Composites

— Aniruddh Vashisth

Paper 6gq: Charge Transport in Self-Assembled Biomolecular Systems — Bo Li, Charles M. Schroeder

Paper 6gu: Chiral Nanomaterials Design for Human Health

— Jihyeon Yeom

Paper 6gx: Functional Nanomaterials Via Self-Assembly: Theory and Simulation

— Hessam Malmir

Paper 6gy: Rational Synthesis and Assembly of Doped Nanomaterials for Quantum and Optoelectronic Applications

- Matthew Crane

Paper 6gz: Designing Nanomaterials and Electronic Devices for Multi-Level Neural Interfacing

— Huiliang Wang

Paper 6hb: Liquid Metal Encapsulation: Towards Next Generation Flexible Electronics

- Megan A. Creighton

Paper 6kb: Design of Flow Reactors and Functional Nanomaterials for Energy & Photocatalytic Applications

— Ioannis Lignos

Paper 6gg: Multi-Sensor System for Complex Chemical Environment Detection

— Yixin Liu

Paper 6kh: Nanotechnology and Neurotoxicity: Exposure to Ultrafine (nano) Particles and its Impact on the Human Brain: Case Studies for Cooking and Diesel Engine UFPs

— Mehdi Amouei Torkmahalleh

Paper 6gt: Evaluation of the Influence of Ce₄ */Ce₃ * Redox-Couple on the Cyclyc Regeneration of NiO-PdO/CeO₂ Nanoparticles for Asphaltene Steam Decomposition

— Oscar Medina

Paper 6gk: Beyond Lithium Aqueous Electrochemical Energy Storage

- Daniel S. Charles

Paper 6gl: Interfacial Engineering of 2D Nanomaterials for Biomedical and Energy Application

— Dorsa Parviz

Paper 6ha: Understanding of Nanoparticle Self-Assembly Mechanisms and Its Applications to Energy Storage and Bio-Medical Applications

- Jaewon Lee

Paper 6gc: Colloidal Electronic Cells As Building-Blocks for Synthetic, Tissue-like Scaffolds

— **Albert Tianxiang Liu**, Michael Strano

Paper 6gh: Enhancement Routes of Corrosion Resistance in Steel-Reinforced Concrete By Using Nanomaterials — Arash Etemad

Paper 6gr: Eco Friendly Strategies for Nanocellulose Production Using a Non Commercial Enzymatic Cocktail

— **Paula Squinca**, Stanley Bilatto, A. C. Badino, Cristiane Sanchez Farinas

Paper Gas: Interfacial Molecular

Paper 6gs: Interfacial Molecular Engineering of Bio-Inorganic Systems from Aqueous Molecules to Assembled High Order Functional Materials

Tyler D. Jorgenson
 Paper 6gv: Meet the Faculty: Investigating the Properties of Nanoparticles

Containing Fullerene-like Molecules

— Kimberly Bowal, Jacob W Martin,
Laura Pascazio, Markus Kraft

Paper 6gw: Recombinant Peptide-Templated Palladium Nanoparticle Synthesis and Their Catalytic Activity in Coupling Reactions

— Imann Mosleh, M. Hassan Beyzavi, Robert Beitle

Paper 174ae: Plant Genome Engineering with Nanotechnology for Agricultural Applications

— **Gozde Sultan Demirer**, Huan Zhang, Juliana Matos, Abhishek Aditham, Brian Staskawicz, Markita Landry

Paper 6kv: Synthesis and Characterization of Perovskites — Atefe Hadi

Paper 6ky: Development of Nanoscale Imaging Tools to Understand Complex Biomolecular Dynamics

– Yang Zhang

Paper 6Id: Scalable Electronic Separation of Single-Walled Carbon Nanotubes (SWCNTs) via Novel Chromatographic Methods

— **Payam Rezaei**, Lisa Pfefferle, Douglas D. Frey

■ PARTICLE TECHNOLOGY

Paper 6hc: Mechanical Programming of Granular Materials in Hydrogels for Tissue-like Behaviors

— **Yin Fang**, Heinrich M. Jaeger, Bozhi Tian

Paper 6hd: Dynamics of Carbonaceous Nanoparticles: Climate Impact & Fire Detection

- Georgios A. Kelesidis

Paper 6he: Particle Simulation in Rotating Reactors

- Dan Sun

PHARMACEUTICALS

Paper 6hf: Development of Strategies to Combat Genomic Instability in Cell Culture Engineering, Biopharmaceutical Production, Disease and Ageing

— Philipp Spahn

Paper 6hi: Engineering Lipid and Polymer-Based Nanomaterials for Drug, Protein and Gene Delivery

— Yamin Li

Paper 6hk: Reengineering the Tumor Microenvironment to Alleviate Hypoxia, Increase Drug Delivery and Enhance Immunotherapy

- John D. Martin

Paper 6hj: Priming the Innate Immunity Using Nanomedicine

— Fan Zhang

Paper 6hg: Zwitterionic Polymeric Platforms for Biologic Drug Delivery and Tissue Engineering

— Caroline Tsao, Shaoyi Jiang

POLYMERS

Paper 6hl: Mechanisms of Diffusion in Associative Polymer Networks: Evidence for Chain Hopping

— **Peter Rapp**, Ahmad Omar, Bradley Silverman, Zhen-Gang Wang, David A. Tirrell

Paper 6hm: Programmable Deformation and Assembly of Soft Active Materials

— Ji-Hwan Kang

Paper Ghn: Molecular-Based Modeling of Polymer Dynamics for Material Design and Processing

— Marat Andreev

Paper 6hp: Molecular—Scale
Engineering of Charge—Containing
Polymers and Electrochemical Interfaces
— Snehashis Choudhury

Paper Ghr: Optimizing the Properties of Advanced Materials through Molecular Design

— Bassil El-Zaatari

Paper 6hs: Polymer Mechanochemistry in Molecular Machines and Medical Treatments

— Qiong Wu

Paper 6hu: Microfluidic Processes to Engineer Hydrogel Particles and Their Applications in Biomedical Engineering — Jae Jung Kim

Paper 6hv: Functional Polymers for Molecular and Materials Design

- Alice B. Chang

Paper 6hz: Towards Sustainable Polymers through Integration of Dynamic Covalent Chemistry and Advanced Processing

- Kailong Jin

Paper Gic: Specialized Polymers for Integrating Advanced Synthetic and Biological Materials

- Jeffrey M. Ting

Paper 6id: 3D Printed Reconfigurable Liquid Crystal Elastomers Via Dynamic-Covalent Bonds

— Emily Davidson

Paper 6ie: Granular Composite-Enabled Multi-Scale Dynamic Responsive Materials

— **Yin Fang**, Endao Han, Yuanwen Jiang, Yiliang Lin, Xianghui Xiao, Jin Wang, Heinrich M. Jaeger, Bozhi Tian

Paper Gif: Multiscale Modeling and Enhanced Sampling to Probe Peptide and Peptidomimetic Assemblies

Janani Sampath, Jim Pfaendtner
 Paper 6ko: Exploring the Structure of

Gradient Double Network Gels

— Pandiyarajan Chinnayan Kannan

Paper 6hw: Engineering the Molecular Packing Autonomously

— Jie Xu

Paper 6ho: Sustainable Approaches to Polymer Recycling

— Michael Miranda

Paper 6hq: Structure-Property-Dynamics Relationships in Multi-Phasic Polymers: Leveraging Self-Assembly of Compatibilizers

— Avanish Bharati

Paper 6hx: Functional Materials Design Guided By Polymer Physics

— **Renxuan Xie**, Michael L. Chabinyc, Ralph H. Colby, Enrique D. Gomez

Paper 6hy: Mechanics and Processing of Polymeric Materials for Soft Electronics and Robotics

- Samuel E. Root

Paper 6ib: Design and Synthesis of Microporous and Nanoporous Polymer Domains for Separation and Purification Processes

— Mahdi Mohammadi Ghaleni

■ PROCESS DESIGN, DEVELOPMENT, & CONTROL

Paper 6ig: Accelerating Chemical Discovery and Process Development with Theoretical Models and Machine Learning

— Hanyu Gao

Paper 6ii: Systems Approach to Advanced Decision-Making in Chemical Engineering, Biomanufacturing, and Society

— Yu Luo

Paper 6ik: Leveraging Scale-Appropriate Principles of Metal-Oxide Reaction Engineering and Particle Technology Science for Energy Conversion Solutions

- Mandar Kathe

Paper 6il: Online Process Optimization of Complex Cyber-Physical Systems

- Dinesh Krishnamoorthy

Paper 6in: Process Control and Developpement for Energy-Efficient Applications

— Esma Ines Achouri

Paper 6kf: Uncertainty Quantification and Risk-based Decision Support Methodologies for Healthcare and Advanced Manufacturing

— **Francesco Rossi**, Flavio Manenti, Guido Buzzi-Ferraris, Gintaras Reklaitis

Paper 6ij: Review of Recent Trends in Sulfur Unit Capacity Expansion Projects — Avinashkumar Karre

Paper Gio: Modelling of Gas Recovery from South African Shale Reservoirs

— Diakanua Nkazi, Thembinkosi

Paper 6ip: Modeling and Simulation of Modular Refinery for Production of Fuels with Low Environmental Pollution

— Diakanua Nkazi, Mbinzi Kita Deddy Ngwanza Sr.

Paper Gir: Polyphenol-Inspired Coatings for Membrane Surface Engineering

— **Lyuhong Zhang**, Na Zhang, Xiaowei Tantai, Xiaoming Xiao

Paper 6is: 20-Plus Years after the Pioneering Work at the University of Oklahoma-Chemical Engineering: Capillary Condensation of Light Hydrocarbons in MCM-41 Type Nano-Porous Media

— Mariana Ioneva

Paper 6it: Detailed Stress Analysis of Floating Platforms

— David Etemad

Paper 6im: Process Systems
Engineering and Dynamic Process
Control of Large-Scale Systems

— Khalid Rashid

Paper 6ih: CO₂ Utilization through Dry Reforming of Methane Reaction — Shaik Afzal. Nimir Elbashir.

Paper 6la: Process Systems

Mahmoud El-Halwagi

Engineering (PSE)

— Ravendra Singh

SEPARATIONS

Paper 6iv: Gas Hydrates Research: From Fundamental Science to Engineering Applications

— Ahmad Abdul Majid

Paper 6iw: The Design, Synthesis and Testing of Advanced High-Performance Ionene Polymers As Gas Separation Membranes

— **Irshad Kammakakam**, Jason E. Bara Paper 6iz: Hybrid Membranes for Challenging Energy Separations — Yang Liu

Paper 6ja: Advanced Membranes for Sustainable Separations at the Water-Energy Nexus

– Oishi Sanyal

Paper 6jb: Rational Design of Nanofiltration Membranes for the Removal of Trace Organic Contaminants from Waste Water Based on Single-Molecule Dynamics and Heterogeneity — Daniel Kienle, James S. Weltz, Andres Chaparro Sosa, Rebecca

Paper 6jc: Membrane Materials and Transport Studies for Sustainable Water, Energy and Life Sciences: From Fundamentals to Applications

Falatach, Joel L. Kaar, Daniel K.

— Ngoc Bui

Schwartz

Paper 6jn: Biomimetic and Polymeric Membranes for Enhanced Selectivity in Desalination and Ionic Separations — Jay R. Werber

Paper 6jo: Solution-Processing Chemistry: Making New Adsorbents, Catalysts and Composite Materials for Clean Energy Applications

- Zhigang Hu

Paper 6jf: Specific Cake Resistance As a Vital Index for Sustainable Water Solutions

— **Mutiu Kolade Amosa**, Tamrin Bin Tajari, Fatai Alade Aderibigbe, Mohammed Saedi Jami

Paper 6jg: Comparative Studies of Silica Gel and MCM-41 after Modifications for Carbon Dioxide Adsorption at High Temperature

— Dinesh Kumar

Paper 6jh: Application of MOFs As Adsorbents in the Field of C₈ aomatics Adsorption Separation — Lunxi Li

Paper 6ji: Biosorption of Methylene Blue Using Citric Acid Modified Arjun Bark Powder

— Dilip Mondal, Shyamal Roy

— Canghai Ma

Paper 6jj: Next-Generation Molecularly Selective Materials and Processes for Scalable Energy Efficient Separations

Paper 6jk: Enhancement of CO₂ Absorption from Gas Streams Using Nanofluids in Hollow Fiber Gas–Liquid Membrane Contactor

— Seyed Mojtaba Mirfendereski

Paper 6jl: CO₂ Removal Using Highly Permeable, Ultra Thin and Well Oriented SAPO-34 Zeolite Membrane Synthesized By a Novel Four-Step Method

– Seyed Mojtaba Mirfendereski

Paper 6jm: Acoustic Cavitation Induced Chemical Functionalization of Biochar: A Feasible Strategy for Effective Removal of Heavy Metals

— **Baharak Sajjadi**, Wei Yin Chen, Daniell Mattern Paper 6ix: Synthesis of Environmentally Friendly and Sustainable Multi-Functional Surfaces and Interfaces

Sebastian Hernandez

Paper 6jd: Microporous Molecular Sieves for Membrane and Adsorptive Separations

— Shaowei Yana

Paper 6je: Absorption and Desorption Mass Transfer Rates at Elevated Pressure in a Simple Hydrocarbon System

- Michael Miranda

SYNTHETIC BIOLOGY

Paper 6jq: Biomimetic Microelectronic Systems for Deciphering Neurotransmission and Hormone Release

— Sathish Ramakrishnan

Paper 6jr: FSP-DDF Coupling Model of Lbm for the Fluid Flow and Heat Transfer in Porous Media

— Shuyan Wang, Shuren Yang, Ruichao Tian, Baosli Shao, Yujia Chen, Qiji Sun

Paper 6jp: Novel Approaches for Prebiotic Detection and Control of Microbial Communities

– Fatima Enam

THERMODYNAMICS

Paper 6jw: Protein Condensation in Nature: Functional or Pathological? — Mohammad Safari

Paper 6ju: Thermodynamic Behavior and Thermophysical Properties of Unusual Fluids: Heavy Oils

- Francisco Ramos-Pallares

Paper 6jv: New Data, Sensors and Models to Avoid Cryogenic Solids Formation in LNG Production

- Arman Siahvashi, Saif al Ghafri, Paul L. Stanwix, Brendan F. Graham, Eric F. May

Paper 6jt: Interaction between Indian Coal-Ash and Iron-Ore Using Chemical Looping Combustion

— Gajanan Surywanshi

(7) Public Affairs and AIChE: A PAIC **Town Hall**

Sunday, Nov 10, 3:00 PM Hyatt Regency Orlando, Orlando Ballroom M

Nada Assaf-Anid, Chair

Sponsored by: Public Affairs and Information Committee (PAIC)

3:00 Welcoming Remarks from Session Chair, Nada Anid, New York Institute of Technology

3:05 Paper 7a: RAPID Manufacturing Institute and AIChE

- Phillip R. Westmoreland

3:20 Paper 7b: The Importance of Credentialing and Licensure — Deborah Grubbe

3:35 Paper 7c: Legal Developments

on Plastics: Basel Convention and the Circular Plastics Economy - Mary Ellen Ternes

3:50 Paper 7d: Responding to Paradigm Shifts

- Dale Keairns

(8) 3D Printing Applications in Catalysts, Reactions, and Energy Industry

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Bayhill 28 Lin Li, Chair

Kuochen Tsai, Co-Chair Azita Ahmadzadeh, Co-Chair

Sponsored by: 3D Printing

- 3:30 Paper 8a: Demystifying Mass Transfer in Electrolyzers through Rapid Prototyping with 3D Printed Parallel Plate Cells
- Stéphane Weusten, Luc Murrer, Mattheus de Groot, John van der Schaaf
- 3:52 Paper 8b: Additive Manufacturing of Catalyst Support Structures with in Operando Adjustable Mass Transport and Flow Characteristics
- Sebastian Trunk, Giang Do, Wilhelm Schwieger, Hannsjörg Freund
- 4:14 Paper 8c: Role of 3D Printed and LED-Driven Photostation in Photocatalytic and Photo-Fenton Activity of Iron Oxide Doped Graphitic Carbon Nitride
- Mathew M. Desipio, Dipendu Saha
- 4:36 Paper 8d: Solution-Based 3D Printing of Hierarchical Microporous Polymers for Energy-Efficient Adsorption - **Fengyi Zhang**, Yao Ma, Jianshan Liao, Victor Breedveld, Ryan Lively
- 4:58 Paper 8e: Titanium/Titania Electrocatalyst for Hydrogen Evolution Synthesized Via a Combination of 3D Printing and Anodization
- Patricia Taboada-Serrano, Xiang Li, Costas Tsouris
- 5:20 Paper 8f: Advanced Manufacturing Enabling Process Intensification for Catalytic Processes - Matthew S. Ide, Changmin Chun, Anastasios Skoulidas, William A.
- 5:42 Paper 8g: 3D-Printed Reactor in Methanol Steam Reforming

- Zhuangdian Liang

Lamberti, Dave Dankworth

(9) Active Colloidal Systems Sunday, Nov 10, 3:30 PM

Hyatt Regency Orlando, Plaza International Ballroom J Christopher L. Wirth, Chair Mark Kastantin, Co-Chair Ubaldo M. Córdova-Figueroa, Co-Chair

Sponsored by: Interfacial Phenomena

- 3:30 Paper 9a: Light-Switchable Active Particles: From Pulling to Pushing, from Fusion to Fission
- Hanumantha Rao Vutukuri, Jan Vermant
- 3:45 Paper 9b: Hydrodynamic Interactions between Microswimmers Trapped at Interfaces
- Nicholas G. Chisholm, Kathleen J. Stebe

4:00 Paper 9c: Propulsion of Asymmetric Dielectric Particles Under High Frequency AC Electric Fields

— Xingfu Yang, Jingjing Gong, Ning Wu

4:15 Paper 9d: Collective Dynamics of Polarizable Active Particles Under Confinement

- Javier D. Gomez. Gerrit Gaillard. Carlos Silvera Batista

4:30 Paper 9e: Axisymmetric Spheroidal Squirmers and Self-Diffusiophoretic Particles

- Ruben Poehnl, Mihail N. Popescu, William E. Uspal

4:45 Paper 9f: Displacement Fields Around Thermally Forced and Active Colloids at Interfaces

- **Mehdi Molaei**, Jiayi Deng, Nicholas G. Chisholm, John C. Crocker, Kathleen Stebe

5:00 Paper 9g: Shape-Directed Assembly of Active Colloidal Crystals - Allan M. Brooks, Cameron T. Long, Darrell Velegol, Ayusman Sen

5:15 Paper 9h: Controlling Active Brownian Motion By State-Dependent **Rotational Diffusion**

- Miguel Angel Fernandez Rodriguez, Fabio Grillo, Laura Alvarez-Frances, Marco Rathlef, Ivo Buttinoni, Giovanni Volne Lucio Isa

5:30 Paper 9i: Autonomous Navigation of Colloidal Robots Via Shapeshifting — Yong Dou, Kyle J.M. Bishop

5:45 Paper 9j: Bayesian Inference and Design for Acoustic Levitation and Propulsion

- Kiran Dhatt-Gauthier

(10) Advanced Materials for **Carbon Dioxide Capture for Power** Generation

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Challenger

David Hopkinson, Chair Lingxiang Zhu, Co-Chair

Sponsored by: Advances in Fossil **Energy R&D**

3:30 Paper 10a: Process Optimization Using Perturbation Expansion Solutions for Membrane Gas Separation Modules - Norfamila Che Mat, Glenn

Lipscomb

3:49 Paper 10b: Novel Microwave-**Enhanced Non-Aqueous Slurry Process** for Post-Combustion CO, Capture

— Fan Shi, Tuo Ji, Hari Paudel, Yuhua Duan, Jeffery Culp, Christopher Marin, McMahan L. Gray

4:08 Paper 10c: Low CO. Concentration Post-Combustion Capture: Process Insights

— Reynolds A. Frimpong, Bradley Irvin, Heather Nikolic, Kunlei Liu

4:27 Paper 10d: Process Modeling and Optimal Synthesis of a Fixed Bed System for CO₂ Capture Using a Diamine-Appended Metal-Organic Framework **Ryan Hughes**, Goutham Kotamreddy, Debangsu Bhattacharyya, Michael S. Matuszewski, Benjamin P. Omell, Jeffrey R. Long, Rebecca Siegelman, Stephanie Didas, Surya Parker

4:46 Paper 10e: Highly Polar Polymers with Superior Membrane CO₂/N₂ Separation Properties for Carbon Capture

— Haiqing Lin, Junyi Liu

5:05 Paper 10f: Systematic Atomistic Simulations of CO, and N, Permeabilities in Polymers

- Wei Shi, Lingxiang Zhu, Surendar Venna, Kevin P. Resnik, David Honkinson

5:24 Paper 10g: Preparation of FAU Zeolite Membranes on Polydopamine Modified Al₂O₂ Tubes for Dewatering of Amine-Based Post-Combustion CO₂ Capture Solutions

- Feng Zhu, James Landon, Kunlei Liu

5:42 Paper 10h: Nitrogen-Doped Graphene Oxide Quantum Dot Membranes for CO₂ Capture Fanglei Zhou, Huynh Ngoc Tien, Weiwei Xu, Qiaobei Dong, Shangwen Zha, Huazheng Li, Dinesh Behera,

(11) Advanced Modelling and Data Systems Applications in Next-Gen Manufacturing

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Bayhill 27 Michael Lovette, Chair Pouria Motevalian, Co-Chair

Sponsored by: Next-Gen Manufacturing

Shiguang Li, Miao Yu

3:30 Paper 11a: Collaborative Simulation Development Accelerated By Cloud Based Computing and Software As a Service Model

— Howard Stamato, Jose E. Tabora, Pablo Rolandi, Vinny Couming, Peter Lyu, Ross Rudow

3:52 Paper 11b: Rational Solvent Selection Guided By Machine Learning and Molecular Descriptors in Asymmetric Catalytic Reactions - Yehia Amar, Artur M. Schweidtmann,

Liwei Cao, Paul Deutsch, Alexei A. Lapkin

4:10 Paper 11c: Application of Multivariate Statistical Process Control to a Drying Process for Continuous Pharmaceutical Manufacturing - Chikara Tsujikwa, Sanghong Kim, Takuya Nagato, Masaru Serizawa, Shinji

4:28 Paper 11d: Multivariate Data Analysis to Drive Process Understanding and Optimization

- **Sagar Harinarayan**, Lorcan Brennan, Guangyang Hou, Deep Golwala, Justin O'Sullivan, Damian Duffy

Hasebe

- 4:46 Paper 11e: Dissolution Prediction By Process Analytical Technology, Machine Learning and Mathematical Modeling: Toward the Real-Time Release Testing of Pharmaceuticals — Brigitta Nagy, Dorian Galata, Attila Farkas, Botond Szilagyi, Qinglin Su, Zoltan K. Nagy, Zsombor K. Nagy
- **5:04 Paper 11f:** An Integrated Approach to Modelling, Data, and Control for Pharmaceutical Manufacturing
- Richard D. Braatz
- **5:24** Paper 11g: Combining Big Data Analytics and Computational Chemistry in Target-Based Drug Discovery — Petar Zuvela, J. Jay Liu
- **5:42 Paper 11h:** Utilizing Data Systems and Modeling to Evaluate Equipment Fit and Technical Capabilities in External Drug Substance Manufacturing
- Whitney Nikitczuk, Brendan C. Mack, Buck Holloway, Daniel Perkins, Joshua Lavender, Christopher Wilbert

(12) Advances in Enzymatic Catalysis Sunday, Nov 10, 3:30 PM

Hyatt Regency Orlando, Florida Ballroom A

Andrew J Adamczyk, Chair Jiafu Shi, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30** Paper 12a: Development of Multi-Enzyme Immobilized Biocatalytic Processes for Synthesis of Small Molecule APIs
- **Rachel S. Bade**, Jacob H. Forstater, Shane T. Grosser, James P. Corry
- **3:48** Paper 12b: Computational Exploration of Peptide Hydrolysis By Serine Protease: Combined Reaction Path and Process Variable Analysis Ashraf Ali, Ashley Caroline Massey, Shounak Datta, Andrew J Adamczyk
- **4:06** Paper 12c: Cooperative Catalysis for Selective Oxidation with Hybrid Gold Nanoparticle Enzyme Materials

 Chimmey Vorma, Joseph Brindle
- Chinmay Verma, Joseph Brindle, Patrick Nelson, **Michael M. Nigra**
- **4:24** Paper 12d: Combinatorial Experimental and Computational Approaches Facilitate Implementation of Amphiphilic Hydrogels for User-Controlled Enzyme Immobilization
- **Jordan Chapman**, Ahmed E. Ismail, Cerasela Zoica Dinu
- **4:42 Paper 12e:** Structure-Based Prediction and Design of Polypeptide Substrate Specificities of Glycosyltransferases
- **Sai Pooja Mahajan**, Yashes Srinivasan, Jason Labonte, Matthew P. DeLisa, Jeffrey J. Gray
- **5:00 Paper 12f:** Mechanistic Study of Glycyl Radical Enzyme
- **Zhongyue Yang**, Heather J. Kulik

- **5:18** Paper 12g: Structure-Function Relationships in Cooperative Biocatalysis By Multi-Enzyme Assemblies
- Mason Smith, Prabhu Ponnandy, Fei Wen
- **5:36** Paper 12h: Expanding the Utility of Amine Dehydrogenases Toward the Biocatalytic Production of Chiral Amines
- Robert D. Franklin, Conner Mount, Umair Alvi, Bettina Bommarius, Andreas S. Bommarius

(13) Atomistic and Molecular Modeling and Simulation of Polymers Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 8 Brett Savoie, Chair

Sponsored by: Polymers

Li Xi, Co-Chair

- **3:30 Paper 13a:** Chemical and Mechanical Stability of a Model Ionic Liquid Epoxy Material Exposed to Galactic Cosmic Ray in a Simulated Martian Environment
- **Sasan Nouranian, Alireza Asiaee**, Farzin Rahmani, Shan Jiang, Alexander Lopez, Hunain Alkhateb
- **3:45** Paper 13b: An Intermittent QM/ MM Technique to Model Force Induced Bond Scission in Polymeric Systems — Kevin R. Hinkle
- **4:00** Paper 13c: Study of Orientational Dynamics in a Cross-Linked Epoxy Network Using Atomistic Simulations Ketan S. Khare, Frederick R. Phelan Jr.
- **4:15 Paper 13d:** Polymer Electrolytes for Battery Technology
- Janna K. Maranas
- **4:45** Paper 13e: Machine-Learning on the Coarse-Grained Polymer Genome *Michael Webb*, *Nicholas Jackson*, *Juan de Pablo*
- **5:00 Paper 13f:** Biased Sampling of 3D Polymer Conformations in an External Field Using Brownian Bridges
- **Shiyan Wang**, Doraiswami Ramkrishna, Vivek Narsimhan
- **5:15 Paper 13g:** Developing a Tractable Simulation of Primary Crystal Nucleation in a Polymer Melt
- **Douglas R. Tree**, Pierre Kawak, Andrew Gibson, Beverly Delgado
- **5:30 Paper 13h:** Simulation of Peg/Poly Aspartic Acid Micelles Provides Insight for Design of Drug-Delivery Systems
- Rainier Barrett, Andrew White
- **5:45** Paper 13i: Prediction of Self-Diffusion Coefficients of Polymer Melts Using Modified Free Volume Theory and MD Simulation
- Chi Pui Jeremy Wong, Phillip Choi

(14) Biomaterials and Life Science Engineering: Faculty Candidates I Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 7 Mark W. Tibbitt, Chair

Whitney L. Stoppel, Co-Chair Handan Acar, Co-Chair Audie Thompson, Co-Chair

Sponsored by: Biomaterials

- **3:48 Paper 14a:** Custom-Built Polymers Promote Stabilization, Delivery, and Bioavailability in Precision Drug Formulation Strategies
- **Jeffrey M. Ting**, Frank S. Bates, Theresa M. Reineke, Matthew V. Tirrell
- **4:06 Paper 14b:** Engineering Biomaterials to Recapitulate the Stem Cell Microenvironment
- Christopher M. Madl
- **4:24 Paper 14c:** Liquid Infused-Elastomers As a Multi-Functional Material in Implantable Bioelectronics
- **Alexandra Rutz**, George Malliaras
- **4:42 Paper 14d:** Rapid Actuation and Tunable Control of DNA-Based Mechanisms
- Alexander E. Marras, Carlos E. Castro
- **5:00 Paper 14e:** Biomimetic Production of Polymer Fibers from Reversibly Cross-Linked Polysaccharide Networks in Water
- **Crystal K. Chu**, Alby Joseph, Suman Bose, Robert Langer, Daniel G. Anderson
- **5:18 Paper 14f:** Designer Biomaterials and Integrated Platforms Toward Precision Medicine
- Jouha Min
- **5:36 Paper 14g:** Mechanophore-Based Biomaterials for In Vivo Ultrasound-Triggered Light Generation
- **Qiong Wu**, Gun Kim, Abigail Halmes, Shang Ning, Clair Lundberg, Michael Oelze, King Li, Jeffrey Moore
- **5:54** Paper 14h: Present and Future of Bioinspired Phenolic Coatings for Surface and Interfacial Engineering *Kyueui Lee*

(15) Biomimetic Materials I

Sunday, Nov 10, 3:30 PM
Hyatt Regency Orlando, Celebration 5
R. Helen Zha, Chair
Neha Kamat, Co-Chair
Marjan Rafat, Co-Chair

Sponsored by: Biomaterials

Xi Chen, Co-Chair

- **3:30 Paper 15a:** Progelator Peptides and Peptide-Polymer Conjugates for Treating Myocardial Infarction
- **Nathan Gianneschi**, Karen L. Christman
- **4:06** Paper 15b: Light-Responsive Fluorescently-Labeled Cyclic Peptides for Selective and Reversible Labeling of Therapeutic Cells
- John Schneible, Ashlyn Young, Vladimir Pozdin, Donald Freytes, Michael Daniele, **Stefano Menegatti**

- **4:24 Paper 15c:** Investigating Sequence Effects on the Biodegradation of Peptoid Substrates
- **Mariah J. Austin**, Hattie C. Schunk, Adrianne M. Rosales
- 4:42 Paper 15d: Self-Assembled Tri-Peptides As Water-Responsive Materials — Roxana Piotrowska, Travis Hesketh, Alan Martin, Deborah Bowering, Haozhen Wang Wang, Chunhua T. Hu, Chunqiu Zhang, Scott McPhee, Tong Wang, Yaewon Park, Pulkit Singla, Tell Tuttle, Rein Ulijn, Xi Chen
- **5:00** Paper 15e: A Kinetic Path to Hierarchically Organized Soft Materials from Self-Assembling Discotics

 Michael VandenBerg, Matthew
- Michael VandenBerg, Matthew Webber
- **5:18** Paper 15f: Nanoparticles Self-Assembly for the Preparation of Bioinspired Materials with Stimuli-Responsive Color Changing Ability
- Responsive Color Changing Ability
 *Marco Lattuada*5:36 Paper 15g: Protein-Engineered
- Hybrid Nanomaterials with Complex Morphologies
- Won Min Park

(16) Biomolecules at Interfaces I

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom K Yeongseon Jang, Chair Peter J. Beltramo, Co-Chair Erick S. Vasquez, Co-Chair

Sponsored by: Interfacial Phenomena

- **3:30 Paper 16a:** Reagentless DNA Bioconjugation to Metal Surfaces *Ariel Furst*
- **3:45 Paper 16b:** Single Molecule Studies of Ionic Strength Effects on Interfacial DNA Searching and Hybridization
- **Jeremiah Traeger**, Daniel K. Schwartz

Chih-Chen Hsieh

- **4:00** Paper 16c: Diffusive Behavior of DNA Adsorbed on Lipid Bilayers Supported on a Glass Substrate *Chieh-Jung Lee*, *Po-Hsiang Wang*,
- **4:15 Paper 16d:** Reorientation of Cytochrome c on Silica Nanoparticles Induced By pH
- **Yao Wu**, Jens Meissner, William A. Shelton Jr., Gerhard H. Findenegg, Bhuvnesh Bharti
- **4:30 Paper 16e:** Membrane Outer Leaflet Is the Primary Regulator of Membrane Damage Induced By Silica Nanoparticles in Vesicles and Red Blood Cells
- **Saeed Nazemidashtarjandi**, Amir M. Farnoud
- **4:45** Paper 16f: Sculpting Vesicles with Active Particles: Less Is More

 Hanumantha Rao Vutukuri, Jan
- **5:00 Paper 16g:** Loss of Membrane Asymmetry Alters the Interactions of Red Blood Cells with Nanoparticles
- Parnian Bigdelou, Amir M. Farnoud

- **5:15** Paper 16h: Protein Adsorption on Phospholipid Polymer Interfaces: The Effect of Chain Length and Its Hydration Structure
- **Toshinori Shimanouchi**, Tomohiro Nakayama, Yukitaka Kimura
- **5:30 Paper 16i:** Influence of Porous Materials on Amyloid- β Protein Aggregation
- Michael Lucas, Benjamin K. Keitz

(17) Biotechnological Production of Food and Feed Ingredients

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 1 Hesham Ali El-Enshasy, Chair Nuttha Thongchul, Co-Chair Jianxin Sun, Co-Chair

Sponsored by: Food

- **3:30 Paper 17a:** Selective Enrichment of Oat Groats Using Chemical-Free Electrostatic Separation
- Dinara Konakbayeva, **Solmaz Tabtabaei**
- **3:48** Paper 17b: Fungal Treatment to Enhance the Nutritional Value of Canola Meal for Animal Feed
- Fatemeh Heidari
- **4:06** Paper 17c: Pectinase Production By Aspergillus Niger in Submerged Cultivation Using Statistical Optimization Approach
- **Elsayed A Elsayed**, Hamiza Suhaimi, Roslinda Abd Malek, Hesham EL Enshasv
- **4:24 Paper 17d:** Evaluation of Microwave Irradiation Effect on Reaction, Separation (ATPS) and Simultaneous Reaction-Separation of Galactooligosaccharides (GOS) Production
- Germán Castro Sr., Juan Serrato
- **4:42 Paper 17e:** Interactive Effect of Temperature, Light Quality and Intensity on Algae Growth and Nutrient Composition
- Xiangpeng Li, Tyler Johannes
- **5:00** Paper 17f: Scale-up of Protist-Facilitated Biotechnology for Transporting Agrochemicals and Beneficial Bacteria Along Plant Roots
- **Christopher J. Hawxhurst**, Jamie Micciulla, Daniel J. Gage, Leslie M. Shor
- **5:18 Paper 17g:** Keynote: Overproduction of Essential Aromatic Amino Acids in *Synechocystis* sp. PCC 6803
- Arnav Deshpande, Jeremiah Vue, **John A. Morgan**
- (18) Carbon Nanofibers and Related Structures from Renewable and/ or Cheap Feedstock and Their Applications

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Discovery 44 Evan J. Granite, Chair Ioannis Zuburtikudis, Co-Chair

Sponsored by: Carbon Nanomaterials

- **3:30 Paper 18a:** Producing Cleaner Fuels Using Carbon Nanofibers Prepared from a Lignin/Recycled-PET Blend
- **Efstratios Svinterikos**, Ioannis Zuburtikudis, Mohamed Al Marzougi
- **3:55 Paper 18b:** Carbon Nanotube Carpet Growth on Nontraditional Substrates Using an Industrial Gaseous Waste As a Feedstock
- **Aaron Porter**, Xu Li, Placidus B. Amama
- **4:20 Paper 18c:** Carbon Nanofibers and Other Carbon Nanostructures As Carriers of Green Solvents (Ionic Liquids) for the Pretreatment of Saline Water for Desalination
- **Ioannis Zuburtikudis**, Inas M. Alnashef, Hadil AbuKhalifeh, Botagoz Zhuman, Efstratios Svinterikos
- **4:45** Paper 18d: Production of CNT Yarns from Methane Gas for Use As Filaments in Incandescent Bulbs: Effect of Hydrogen Co-Feeding on the Properties of As-Spun CNT Yarns
- **Ezinne Igbokwe**, Michael Daramola, Sunny lyuke
- **5:10 Paper 18e:** Nanophotonic Materials for Low Cost Solar Desalination
- **Ibrahim Abdallah**, Ruikun Xin, Qilin Li
- **5:35 Paper 18f:** Brief Review of Thermal Graphitization of Coals and Carbons
- Evan J. Granite

(19) Cell Biomechanics and Adhesion Sunday, Nov 10, 3:30 PM

Hyatt Regency Orlando, Celebration 3 Roman Voronov, Chair Esther Gomez, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30 Paper 19a:** Matrix Stiffness and Ligand Guide Schwann Cell Phenotype Specification
- Zhenyuan Xu, Greg M. Harris
- **3:48 Paper 19b:** Cellular Adaptations Against Hydraulic Resistance Towards Higher Motility
- **Kaustav Bera**, Adrianna Boen, Pranav Mehta, Panagiotis Mistriotis, Konstantinos Konstantopoulos
- **4:06** Paper **19c:** The Effect of Rigid Red Blood Cells on Platelet Adhesion in Blood Flow: Potential Implications in Sickle Cell Disease
- Alison Banka, Mario Gutierrez, Mark Shamoun, Tyler Tanski, Omolola Eniola-Adefeso
- **4:24** Paper 19d: Dual Role of VWF A₂
 Domain in Regulating VWF Molecular
 Size and Thrombus Growth in Circulation
- **Sriram Neelamegham**, Changjie Zhang, Anju Kelkar
- **4:42** Paper 19e: Identification of Rigid Red Blood Cell Population Rigidity in Sickle-Cell Disease Patients Using a Parameterization Model of Ektacytometry
- **Mario Gutierrez**, Mark Shamoun, Tyler Tanski, Omolola Eniola-Adefeso

- **5:00** Paper 19f: Confined Cell Migration Induces Nuclear Volume Expansion and Blebbing By Triggering RhoA-Mediated Nuclear Influx
- Emily Wisniewski, Panagiotis Mistriotis, Kaustav Bera, Jeremy Keys, Yizeng Li, Soontorn Tuntithavornwat, Robert Law, Eda Erdogmus, Yuqi Zhang, Runchen Zhao, Sean X. Sun, Petr Kalab, Jan Lammerding, Konstantinos Konstantopoulos
- **5:18** Paper 19g: Invited: Nuclear Mechanics in Cell Migration and Tissue Development
- Tanmay Lele

(20) Charged Polymers for Membrane-Based Water and Energy Applications

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Barrel Spring II Geoffrey M. Geise, Co-Chair Piran Kidambi, Co-Chair Milad R. Esfahani, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30 Paper 20a:** Next Generation Charged Poly(arylene ether sulfone) Membranes: Integrating Fouling Resistance, Chlorine Tolerance, and Water/Salt Permselectivity
- Matthew D. Green, Yi Yang
- **3:50 Paper 20b:** Self-Assembling Random Zwitterionic Copolymers As Charge-Selective Nanofiltration Membranes
- Samuel Lounder, Ayse Asatekin
- **4:10 Paper 20c:** Complex Multicomponent Transport through Polymeric Membranes
- **Breanna M. Dobyns**, Bryan S. Beckingham
- **4:30** Paper 20d: Thermodynamics of Ion and Water Uptake in Phase-Separated Ion-Exchange Membranes *Andrew Crothers*, *Robert Darling*, *Ahmet Kusoglu*, *Clayton J. Radke*, *Adam Weber*
- **4:50 Paper 20e:** Functionalized Nanoporous Ceramic Membranes Towards Low-Cost Electrodialysis
- **Greg Newbloom**, Ryan Kingsbury, Rachel Malone
- **5:10** Paper **20f**: High Temperature Proton Exchange Membrane Based on Polycation Polybenzimidazole Blends *Gokul Venugopalan*, *Christopher*
- G. Arges
- **5:30 Paper 20g:** Integrating a CO₂-Selective Membrane Process into a Solid Oxide Fuel Cell System to Enhance H₂ Utilization
- Kai Chen, Witopo Salim, Yang Han, Michael Gasda, W.S. Winston Ho

(21) Chemical Angels Network (CAN) Session: Entrepreneurship & Investing in Early-Stage Chemical Companies

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom N Mark Vreeke, Chair William Byers, Co-Chair

Sponsored by: Entrepreneurship in Chemical Engineering - Sponsored by CIEE

- **3:30 Paper 21a:** Angel Investing in the Hard Sciences Chemical Angel Network (CaN)
- Mark Vreeke
- **3:45 Paper 21b:** "Why I'm an Angel" Panel
- William Byers, Hugh James, Sid White, Jeff Gish
- **4:35** Presentations by Early Stage Companies
- 5:45 Concluding Remarks

(22) Engineering in Cancer Biology and Therapy I: Research Tools and Platforms

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 2 Ebong Eno, Chair Shreyas Rao, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30** Paper 22a: Novel Anti-SSTR₂ Antibody-Targeted Therapy for Neuroendocrine Cancers
- Rachael Guenter, Yingnan Si, Seulhee Kim, Dalton Frederick, Rebekah Boos, Herbert Chen, Lufang Zhou, Renata Jaskula-Sztul, X. Margaret Liu
- **3:48** Paper 22b: "Extracellular Vesicles Derived Supported Bilayer As a Platform for Cell Culture to Understand the Interactions between Adipose Stem Cells and Extracellular Vesicles"
- **Johana Uribe**, Han-Yuan Liu, Claudia Fischbach-Teschl, Susan Daniel
- **4:06 Paper 22c:** Evaluating Chemo-Sensitizing Potential of Oxygen Delivery Facilitated By Transfused Polymerized Hemoglobins on Vascularized Solid Tumors
- **Donald Belcher**, Alexander Williams, Pedro Cabrales, Andre Palmer
- **4:24 Paper 22d:** Engineered Bispecific Antibodies for Targeted Inhibition of Cancer Metastasis
- Jamie B. Spangler
- **4:42** Paper 22e: Treatment Resistance Profiling of a Novel Hypoxic Pancreatic Ductal Adenocarcinoma 3D Organoid System
- Gabrielle Wishart, Priyanka Gupta, Giuseppe Schettino, Andrew Nisbet, Eirini Velliou

- **5:00** Paper 22f: A Computational Model of Subtype Interactions in Small Cell Lung Cancer Predicts Factors Controlling Intertumoral Heterogeneity Leonard A. Harris, Samantha Beik, Sarah M. Groves, Alissa M. Weaver, Carlos F. Lopez, Vito Quaranta
- **5:18 Paper 22g:** Invited: Tissue Engineered Cancer Models for Recapitulating the Tumor Microenvironment
- Iman Hassani, Benjamin Anbiah, Nicole Habbit, Bulbul Ahmed, Michael W. Greene, **Elizabeth Lipke**

(23) Feedstock Logistics for Biorefineries

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Regency Ballroom U

Chang Dou, Chair Vicki S. Thompson, Co-Chair Lynn Wendt, Co-Chair

Sponsored by: Sustainable Biorefineries

- **3:30** Paper 23a: Mechanical Properties and Bulk Flow Characterization of Loblolly Pine
- Tiasha Bhattacharjee, Jordan Klinger, Tyler L. Westover, Aaron D. Wilson, Yidong Xia, Wencheng Jin, Hai Huang
- **3:52 Paper 23b:** Experimental Study of Intermediate Storage and Discharge of Compressible Biomass Particulate Solids in a Wedge-Shaped Hopper of Changing Geometry
- **Jordan Klinger**, Tyler L. Westover, Wencheng Jin, Tiasha Bhattacharjee, Yidong Xia, Hai Huang
- **4:14** Paper 23c: An Overview of Storage-Related Changes Occurring in Cellulosic Biomass Under Commercially Relevant Conditions
- William A. Smith, Lynn M. Wendt, Carlos E. Quiroz Arita, Mitchell A. Plummer
- **4:36** Paper 23d: Optimization of National and Regional Bioenergy Feedstock Supplies As Functions of Price and Biorefinery Scale
- **Damon Hartley**, David N. Thompson, L. Michael Griffel, Yingqian Lin
- **4:58** Paper 23e: Quantifying Variability in Life Cycle Environmental Footprints of Biofuel Produced from Forest Residues in the United States
- Kai Lan, Longwen Ou, Stephen S. Kelley, Sunkyu Park, Hoyoung Kwon, Hao Cai, Michael Wana, Yuan Yao
- **5:20 Paper 23f:** Wear and Why? the Role of Ash in Biomass Processing Equipment Wear
- **Vicki S. Thompson**, Jeffrey A. Lacey, John E. Aston, Kyungjun Lee, Jun Qu, Mary Intwan

- **5:42** Paper 23g: Factors Influencing Nutrient Solubilization from Biomass during Hydrothermal Carbonization
 Saeed Vahed Ogramaleki, John
- Saeed Vahed Qaramaleki, John Villamil, **Charles J. Coronella**, Angel Fernandez Mohedano

(24) Fundamentals of Food, Energy, and Water Systems

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Blue Spring I/II Kirti M. Yenkie, Chair Debalina Sengupta, Co-Chair

Sponsored by: Fundamentals

- **3:30 Paper 24a:** Hidden Economic Impacts of Nutrient Runoff from Livestock Waste
- **Apoorva Sampat**, Gerardo J. Ruiz-Mercado, Victor M. Zavala
- **3:51 Paper 24b:** Energy-Water Nexus in Eco-Industrial Park
- Tapas Das
- **4:12** Paper 24c: Electrochemical Processing to Capture Phosphorus from Concentrated Animal Feeding Operations Waste: Experimental and Process Simulation Investigations
- **Zineb Belarbi**, Damilola A. Daramola, Jason Trembly
- **4:33 Paper 24d:** Pore-Scale Effects of Dilute Organic Macromolecules and Nanoparticles to Inhibit Moisture Loss
- **Yi-Syuan Guo**, Diana Tran, Dusan Losic, Leslie M. Shor
- **4:54 Paper 24e:** Process Intensification of the Conversion of Waste Cooking Oil to Fame Using a T- Microreactor
- **Junaid Ahmad**, Nahla Alamoodi, Anas Alazzam
- **5:15** Paper 24f: Simulation and Energy Assessment of Ammonia-Containing Gas Separation and Recovery Process with Ionic Liquids
- **Guoxiong Zhan**, Fei Chang, Shaojuan Zeng, Zengxi Li, Xiangping Zhang

(25) High Pressure Phase Equilibria and Modeling

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom L

Aaron M. Scurto, Chair Kenneth M. Benjamin, Co-Chair

Sponsored by: High Pressure

- **3:30 Paper 25a:** Volume-Based Phase Equilibrium Calculations
- Dan Vladimir Nichita
- **3:47 Paper 25b:** Gibbs Ensemble Monte Carlo Simulations Probing the Miscibility Gap in Water/Hydrogen Mixtures at High Temperatures and Pressures
- Colin Bunner, Mona Minkara, **J. Ilja Siepmann**

- **4:04** Paper 25c: High-Pressure Vapor-Liquid Equilibria of 1-Alkyl-1-Methylpyrrolidinium bis(trifluoromethylsulfonyl)imide lonic Liquids and CO,
- Tugba Turnaoglu, David L. Minnick, Ana R. C. Morais, Donna L. Baek, Robert V. Fox, Aaron M. Scurto, Mark B. Shiflett
- **4:21 Paper 25d:** Solubility of Gases in Brine for Underground Gas Storage Application: Experimental Measurements and Modeling
- **Salaheddine Chabab**, Pezhman Ahmadi, Pascal Theveneau, Christophe Coquelet, Antonin Chapoy, Jerôme Corvisier, Patrice Paricaud, Rod Burgass, Celine Houriez, Elise El Ahmar
- **4:38** Paper 25e: Solubility and Diffusivity for Hydrofluorocarbon and Hydrofluoroolefin Refrigerants in Poe ISO Vg 32 Lubricant Oil
- **Ana R. C. Morais**, Luke D. Simoni, Aaron M. Scurto, Mark B. Shiflett
- **4:55** Paper **25**f: Evolution of Polystyrene Cell Structure during Extrusion Foaming Process By Population Balance Simulation *Zhimei Xu, Jingman Liu, Yuan Zong*

(26) Industrial Applications in Design and Operations

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Bayhill 24 Iiro Harjunkoski, Chair Vishal Mahindrakar, Co-Chair

Sponsored by: Computers in Operations and Information Processing

- **3:30 Paper 26a:** Optimal Scheduling of Copper Concentrate Operations Under Uncertainty
- **Pengfei Cheng**, Pablo Garcia-Herreros, Mangalam Lalpuria, Ignacio E. Grossmann
- **3:49** Paper 26b: Deterministic Global Optimization Approach to Midterm Planning of an Industrial Integrated Petroleum-Petrochemical Facility

 Ariel Uribe-Rodriguez, Pedro M.
- Ariel Uribe-Rodriguez, Pedro M. Castro, Benoit Chachuat, **Gonzalo Guillén-Gosálbez**
- **4:08 Paper 26c:** Power Cycle Design for Optimal Cogeneration
- Caroline Nielsen, Paul I. Barton
- **4:27 Paper 26d:** Modeling and Optimization of a Bubble Column Reactor and Benzene Chlorination Process
- Noriyuki Yoshio, Lorenz T. Biegler
- **4:46** Paper 26e: Demand Side Management of a Steel Plant Incorporating the Maintenance of Eafs with Alternative Operating Modes
- **Pedro M. Castro**, Giancarlo Dalle Ave, Iiro Harjunkoski, Ignacio E. Grossmann
- **5:05 Paper 26f:** Reduced-Order Model for a Large-Scale Real-Time Optimization of a Residue Fluidized Catalytic Cracker
- Andrew Bai, Kai Wu, **Cornelius Mduduzi Masuku**, Jacques
 Niederberger, Fabio S. Liporace, Lorenz
 T. Biegler

- **5:24** Paper 26g: Evaluation of Local Solvers for Flexibility Analysis of Dynamic Pharmaceutical Processes *Daniel Laky, Shankar Vaidyaraman, Salvador García-Muñoz, Carl Laird*
- **5:43 Paper 26h:** Poultry Production Planning with Batch-Lines in the Agriculture Industry
- **Brenno C. Menezes**, Jeffrey D. Kelly, Tareq Al-Ansari

(27) Membranes for CO₂ Capture Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Barrel Spring I W.S. Winston Ho, Co-Chair Xiaoli Ma, Co-Chair Theodore Tsotsis, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30** Paper 27a: A Carbon Molecular Sieve Membrane-Based Reactive Separation Process for Pre-Combustion CO₂ Capture
- Mingyuan Cao, Linghao Zhao, Dongwan Xu, Secgin Karagoz, Patricia Pichardo, Richard J. Ciora, Paul K.T. Liu, Vasilios Manousiouthakis, Theodore Tsotsis
- **3:51** Paper 27b: Enhancing CO₂ Permeability of Cross-Linked Poly(ethylene oxide) By Doping with Crown Ethers and Metal-Organic Frameworks for CO₂ Capture

 Liang Huang, Haiqing Lin
- **4:12** Paper 27c: Highly Selective Hollow Fiber Membranes for Carbon Capture Via in-Situ Layer-By-Layer Surface Functionalization

 Naveen K. Mishra, Jaime C.
- Naveen K. Mishra, Jaime C.
 Grunlan, Benjamin Wilhite
 4:33 Paper 27d: Field Trial of Spiral-
- Wound Facilitated Transport Membrane Module for CO₂ Capture from Flue Gas — Yang Han, Witopo Salim, Kai Chen, Dongzhu Wu, W.S. Winston Ho
- **4:54** Paper 27e: High-Permeance Polymer-Functionalized Graphene Membranes That Surpass the Postcombustion Carbon Capture Target Guangwei He, Kumar Varoon Agrawal
- **5:15** Paper 27f: Facilitated Transport Nanocellulose Membranes Enhanced By Amine Moieties for CO₂ Separation — Davide Venturi, Marco Giacinti Baschetti
- **5:36 Paper 27g:** Enhanced CO₂ Separation Using Water Swellable Polymer/ Amine Functionalized Zinc Oxide Mixed Matrix Membrane
- Rajashree Borgohain, Pradip Das, Bishnupada Mandal

(28) Metabolic Engineering: Biosynthetic Pathway Engineering and Enzymatic Conversion for Bulk Chemicals

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 4 Han Li, Co-Chair Kevin V Solomon, Co-Chair

Sponsored by: Bioengineering

- **3:30** Paper 28a: Development of a Thermophilic Consolidated Bioprocessing *Clostridum Thermocellum* Platform for Ester Production from Cellulose
- **Hyeongmin Seo**, Cong T. Trinh
- **3:48** Paper 28b: Engineering Synthetic, Catabolically-Orthogonal Co-Culture Systems for Enhanced Conversion of Lignocellulose-Derived Sugars to Fuels and Chemicals
- Andrew D. Flores, Apurv Mhatre, E. Zeynep Ayla, Hyun G. Choi, Arul M. Varman, David R. Nielsen, Xuan Wang
- **4:06** Paper 28c: Turing Waste Cooking Oils into High-Value Products By Metabolic Engineering in Yeast and Bacteria *Ya-Hue Soong*, *Na Liu*, *Dongming Xie*
- **4:24** Paper **28d:** Using Biopolymer to Improve Microbial Production of Hydrophobic Compounds
- **Yurou Liu**, Zhen Jie Low, Xiaoqiang Ma, Hong Liang, Anthony J. Sinskey, Gregory Stephanopoulos, Kang Zhou
- **4:42** Paper 28e: Biosynthesis of Styrene and 4-Hydroxystyrene By Exploiting Aromatic Amino Acid Exporter and Biosensors in *Escherichia coli*
- **Zhenghong Li**, Yiyao Zhou, Sweta Gargatte, Xiaonan Wang, Haoran Zhang
- **5:00** Paper 28f: Improving Lactic Acid Production in *Saccharomyces Cerevisiae* Under Low pH By Directed Genome Evolution
- **Yajie Wang**, Vinh Tran, Huimin Zhao
- **5:18** Paper 28g: Enabling Genetic Tools for Engineering Oleochemical Production in *Yarrowia Lipolytica Mark Blenner*

(29) Modeling, Control, and Optimization of Manufacturing Systems

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Bayhill 25 Joel Paulson, Chair Yankai Cao, Co-Chair

Sponsored by: Systems and Process Control

- **3:30** Paper **29a**: Robust Artificial Neural Networks for Nonlinear Model Predictive Control of Multiscale Stochastic Systems
- **Grigoriy Kimaev**, Luis A. Ricardez-Sandoval
- **3:49 Paper 29b:** Self-Optimizing Control of a Continuous Pharmaceutical Manufacturing Plant
- **David P. Piñeiro**, Anastasia Nikolakopoulou, Johannes Jäschke, Truls Gundersen, Richard D. Braatz

4:08 Paper 29c: Integration of Design, Scheduling, and Control of Batch Processes By Model Based Multiparametric Programming
— Baris Burnak, Efstratios N.

Pistikopoulos

- **4:27** Paper 29d: A Systematic Model-Based Approach for the Design and Control of Protein Crystallization — **Moo Sun Hong**, Amos E. Lu, Richard D. Bragtz
- **4:46** Paper **29e**: Real-Time Coordinating of Multiple Conveyor-Belts and Multi-Quality Stockpiles for Tripper Car Positioning in the Mining Field
- Brenno C. Menezes, Jeffrey D. Kelly
- **5:05** Paper **29f**: Multi-Model Based Model Predictive Control of a Rotational Molding Process
- **Abhinav Garg**, Hassan Abdulhussain, Prashant Mhaskar, Michael R. Thompson
- **5:24 Paper 29g:** Multiscale Modeling and Control of Cell Wall Thickness in Batch Pulp Digester
- **Hyun-Kyu Choi**, Joseph Sang-II Kwon
- **5:43** Paper 29h: Modeling and Uncertainty Analysis of Microbial Electrosynthesis of Acetate for Martian Colonization
- **George Makrygiorgos**, Anthony Abel, Aaron Berliner, Adam P. Arkin, Douglas S. Clark, Ali Mesbah

(30) MOFs, COFs, and Porous Polymer Materials

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 12/13

Satish K. Nune, Chair Wei Fan, Co-Chair

Sponsored by: Inorganic Materials

- **3:30 Paper 30a:** Restricting Lattice Flexibility in Polycrystalline Metal-Organic Framework Membrane for Efficient Carbon Capture
- Deepu Babu**, Kumar Varoon Agrawal**
- **3:48 Paper 30b:** Advanced Sorbent Materials for Noble Gas Separation
- Michael Sinnwell, **Praveen K. Thallapally**, Jian Liu, Debasis Banerjee, Sameh Elsaidi
- **4:06** Paper 30c: Competitive and Cooperative Co-Adsorption in Metal Organic Frameworks Materials: The Role of Hydrogen Bonding
- **Kui Tan**, Stephanie Jensen, Yves Chabal, Timo Thonhauser
- **4:24 Paper 30d:** Design of Stratified Metal Organic Frameworks for Chemical Warfare Agent Concentration and Destruction
- Jonathan Ruffley, Isabella Goodenough, Tianyi Luo, Dorian Thompson, Melissandre Richard, Nathaniel L. Rosi, Eric Borguet, J. Karl Johnson

- 4:42 Paper 30e: A Combined Experimental-Simulation Design Approach to Multi-Porous Covalent Organic Frameworks (COFs) — Swapan Das, Tiara Ann Maula, Jeetain Mittal, Srinivas Rangarajan, Mark A. Snyder
- **5:00 Paper 30f:** Jolly Green MOF: Confinement and Photoactivation of Photosystem I in the Metal Organic Framework ZIF-8
- **Tyler Bennett**, Dibyendu Mukherjee, Bamin Khomami
- **5:18** Paper 30g: Engineering Pore Size of Pillared-Layer Coordination Polymers Enables Highly Efficient Adsorption Separation of Acetylene from Ethylene
- Fang Zheng, Lidong Guo, Bixuan Gao, Liangying Li, Zhiguo Zhang, Qiwei Yang, Yiwen Yang, Baogen Su, Qilong Ren, Zongbi Bao
- **5:36** Paper 30h: Controlling Metal Organic Framework Morphology, Polymorphism and Flexibility *Gaurav Giri*

(31) Nanobiotechnology for Sensors and Imaging I

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Discovery 46 Daniel Roxbury, Chair Margaret Bennewitz, Co-Chair

Sponsored by: Bionanotechnology

- **3:30 Paper 31a:** Multifunctional Hydrogel-Coated Gold Nanoshells for Protein Biomarker Quantification
- **Andrew C. Murphy**, Marissa E. Wechsler, Nicholas A. Peppas
- **3:48** Paper **31b**: Surface Effects of Ultrasmall Nanoparticle on Cellular Uptake, Proliferation, and Multipotency of Neural Stem Cells
- **Seungjo (Joe) Park, Yonghyun (John) Kim**, Yuping Bao, Jennifer Sherwood
- **4:06 Paper 31c:** Quantum Capacitance Based Amplified Graphene Phononics for Studying Neurodegenerative Diseases
- Bijentimala Keisham, Akop Seksenyan, Steven Denyer, Pouyan Kheirkhah, Gregory Arnone, Pablo Avalos, Abhiraj D. Bhimani, Clive Svendsen, Vikas Berry, Ankit Mehta
- **4:24** Paper 31d: Rare Earth Element Doped Nanocrystals for Correlative Cathodoluminescence Electron Microscopy Bioimaging (CCLEM)
- **Kerda Keevend**, Michael Stiefel, Lukas Gerken, Martin T. Matter, Inge K. Herrmann
- **4:42** Paper 31e: Effect of Particle Diameter and Magnetic Anisotropy on Magnetorelaxometry and Magnetic Particle Imaging Performance of Immobilized Magnetic Nanoparticles
- **Zhiyuan Zhao**, Nicolas Garraud, David P. Arnold, Carlos Rinaldi

- **5:00** Paper 31f: DNA-Caged Polymer Nanocomposites for Erasable Fluorescence Imaging
 Elizabeth Jergens, *Kil Ho Lee*, *Yixiao Cui, Jessica O. Winter*
- **5:18 Paper 31g:** Tuning the Size and Composition of Manganese Oxide Nanoparticles for Magnetic Resonance Imaging of Breast Cancer
- **Celia Martinez De La Torre**, Jasmine Grossman, Margaret Bennewitz
- **5:36** Paper 31h: One-Step Synthesis of Water-Soluble Ultrasmall Iron Oxide Nanoparticles with Narrow Size Distribution and Their Application for T_1 -Weighted MRI and Potential Drug Delivery

 Pohlee Cheah, Paul Brown, Yongfeng Zhao

(32) New Tools and Applications from Unconventional Synthetic Biology Organisms

Sunday, Nov 10, 3:30 PM
Hyatt Regency Orlando, Celebration 14
Kate E. Galloway, Chair
Oing Sun, Co-Chair
J. Andrew Jones, Co-Chair
Piyush Jain, Co-Chair
Joseph Rollin, Co-Chair
Albert Keung, Co-Chair

Sponsored by: Bioengineering

- **3:30 Paper 32a:** Biological Conversion of Methanol to Organic Acids Using A. niger Strain
- **Ji Eun Lee**, Jong Hyun Yoon, Eun Ji Kim, Shin Sik Choi
- **3:48** Paper 32b: Genetic Engineering of *Pseudomonas Putida* for the Heterologous Production of Polyketides and Non-Ribosomal Peptides
- **Taylor Cook**, Aditya Ailiani, Brian F. Pfleaer
- **4:06** Paper 32c: Transcriptomics Informs Simplified CRISPR/Cas₉ Genome Editing for Humanization of Glycosylation in *Pichia Pastoris*
- **Neil C. Dalvie**, Justin Leal, Charles A. Whittaker, Kerry Routenberg Love, J. Christopher Love
- **4:24** Paper 32d: Rapid Identification of Optimized Plant Growth Promoting Formulations Using Microwell Arrays to Enhance Biofertilizer Production

 Niloy Barua, Ryan Hansen
- 4:42 Paper 32e: Optical Control of Exopolysaccharide Production in Sinorhizobium Meliloti for Studying Biofilm Formation and Water Retention Yongku Cho, Azady Pirhanov, Yi-Syuan Guo, Jessica M. Furrer, Daniel J. Gage, Leslie M. Shor
- **5:00 Paper 32f:** Chassis Engineering of E. coli Nissle 1917 for Live Biotherapeutic Delivery
- **Halimatun Zainuddin**, Yanfen Bai, Fatima Enam, Thomas J. Mansell
- **5:18 Paper 32g:** Synthetic Transcriptional Motifs in Distributed Systems
- Gregory T. Reeves

(33) Panel Discussion: Chemical Process and Product Design Careers in Industry & Academia (Invited Talks)

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Bayhill 17 Kishori T. Deshpande, Chair

Sponsored by: Product Design

3:30 Paper 33a: Presentation By Dr. Shaibal Roy

— Shaibal Roy

3:55 Paper 33b: Presentation By Dr. Dante Simonetti

- Dante Simonetti

4:20 Paper 33c: Presentation By Dr. Bindu Krishnan

— Bindu Krishnan

4:45 Paper 33d: Presentation By Dr. Chris Norfolk

- Chris Norfolk

5:10 Paper 33e: Presentation By Dr. Nyree Mcdonald

- Nyrée V. McDonald

5:35 Paper 33f: Presentation By Dr. Jodie Lutkenhaus

- Jodie L. Lutkenhaus

(34) Polymers in Industry - Rising Stars (Invited Talks)

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 10 Blair Kathryn Brettmann, Chair Narayan Rameesh, Co-Chair

Sponsored by: Polymers

3:30 Paper 34a: Aqueous Rheology of Hydrophobe-Substituted Cellulose Ethers

— **Nikhil Fernandes**, Lyndsay Leal, Alan Nakatani, Emmett Partain, Jennifer Koenig, Janine Stratton

4:00 Paper 34b: My Wonderful and Random Walk through Polymer Science in Industry

— Ann Fornof

4:30 Paper 34c: Design and Synthesis of Emulsion Polymer Dispersions and Resins for Industrial Products with Improved Eco-Footprint

— **Pu Luo**, James Bohling

5:00 Paper 34d: Recent Advances in Low Temperature Cure Electrodeposition Coatings

— Egle Puodziukynaite, Hyun Wook Ro, Craig Wilson, Brian Okerberg, Reza Rock, Jonathan Weis

5:30 Paper 34e: Sustainable Plastics for Food Packaging

- Christopher Thurber

(35) Pyrolysis of Biomass Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom E

Fernando Resende, Chair Hsi-Wu Wong, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 35a: Single-Pot Hydrocarbon Production from Aqueous Phase Pyrolysis Oil Oxygenates Using Multifunctional Red Mud-Supported Nickel Catalysts

— Hossein Jahromi, Foster Agblevor

3:52 Paper 35b: Mapping Reaction Pathways of Biomass Fast Pyrolysis Using Isotopically Labeled Plant Cell Culture

— **Zhongyu Zhang**, Christopher M. Saffron

4:14 Paper 35c: Turning Food Waste into Nitrogen-Doped Bio-Carbocatalyst — *Elvis Ebikade*, *Dionisios G. Vlachos*

4:36 Paper 35d: Comparing Pyrolysis of D-Arabinose and L-Fucose to D-Xylose

— **Ankush Jain**, Arnab Bose, Phillip R. Westmoreland

4:58 Paper 35e: The Mechanism of vXylose Pyrolysis

— **Ali Zolghadr**, Paul Dauenhauer, Chowdhury Ashraf, Jim Pfaendtner

5:20 Paper 35f: Core-Shell Structured ZSM-5/MCM-41 Catalysts for Catalytic Fast Pyrolysis of Biomass

— **Lei Yu**, Oluwole Ajumobi, Vijay T. John, Julia A. Valla

5:42 Paper 35g: Pyrolysis Kinetics of Live and Dead Wildland Vegetation from the Southern United States

— **Elham Amini**, Mohammad-Saeed Safdari, Thomas Fletcher, David R. Weise

(36) Rational Catalyst Design I: Support Effects

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom D Steven R. Saunders, Chair Luke Roling, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 36a: Single Atom Catalysts Supported on Defective Hexagonal Boron Nitride: Stability and Activity for CO Oxidation

— **Roberto Schimmenti**, Manos Mavrikakis

3:48 Paper 36b: Pt/hBN Catalyst Activity for Syngas Production: The Active Role of hBN

— Leonardo Garro-Mena, Keith Hohn

4:06 Paper **36**c: Elucidating the Support Effects of Perovskite Oxides for the Rational Design of Sinter-Resistant Catalysts

— **Kandis Leslie Abdul-Aziz**, Soham Shah, Samuel Sayono

4:24 Paper 36d: Influence of Al-Al Proximity on Metal Ion Exchange in SSZ-13 Zeolite and Strategies to Characterize and Control It

— Sichi Li, Claire T. Nimlos, Casey Jones, Anthony DeBellis, Imke Britta Mueller, Subramanian Prasad, Ahmad Moini, Rajamani Gounder, William F. Schneider **4:42** Paper 36e: Revisiting Effects of Alkali and Alkaline Earth Co-Cation Additives to Cu/SSZ-13 Standard Selective Catalytic Reduction Catalysts — Yanran Cui, Yilin Wang, Eric D. Walter, Donghai Mei, Janos Szanyi, Yong Wang, Feng Gao

5:00 Paper 36f: Two-Dimensional Transition Metal Carbides As Supports for Tuning the Chemistry of Catalytic Nanoparticles for Effective Shale Gas Dehydrogenation

— Yue Wu

5:18 Paper **36g**: Flame Spray Pyrolysis Designed Defective Catalysts for Carbon Dioxide Conversion

— **Emma Lovell**, Jason Scott, Rose Amal

5:36 Paper 36h: Methods of Coating Ceramic Supports with Carbon in the Case of Supported Ni-Based Catalysts Formulations

— **Esma Ines Achouri**, Nicolas Abatzoglou, Jamal Chaouki

(37) Reaction Engineering for Combustion and Pyrolysis

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom F C. Franklin Goldsmith, Chair Bihter Padak, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 37a: Production and Separation of a Low Fragmentation Thermal Naphthalene Pitch

- William Lamie, Mark C. Thies

3:49 Paper 37b: Blue Whirl Phenomenon- a Potential Fuel Flexible and Soot Free Combustion

— Paul M. Anderson, Sampath Gunukula, Dat T. Tran, Ivan C. Lee

4:08 Paper 37d: Degradation Kinetics of a Liquid Mineral Oil

— **Arnab Bose**, Emily A. Heckard, Phillip R. Westmoreland

4:27 Paper 37c: Pyrolysis, Laminar Flame Speeds, and Ignition Delay Times for Isopropyl Nitrate

— **C. Franklin Goldsmith**, Mark Fuller, Nabiha Chaumeix

4:46 Paper 37e: Predicting the Combustion Properties of Hydrofluorocarbon (HFC) Refrigerants Using the Automated Reaction Mechanism Generator (RMG)

— **David Farina Jr.**, Sai Krishna Sirumalla, Nathan Harms, Richard H. West

5:05 Paper 37f: Propane Pyrolysis Facilitated By Phenyl Radicals: A Combined Experimental and Kinetic Modeling Study

- Peng Yu, Hsi-Wu Wong

5:24 Paper 37g: Message Passing Attention Networks for Reaction Rate Estimation

— **Sai Krishna Sirumalla**, Richard H. West **5:43** Paper 37h: A DFT Study of SO₂ Binding on CuO Oxygen Carrier Under Chemical Looping with Oxygen Uncoupling Conditions.

— Turna Barua, Bihter Padak

(38) Reaction Path Analysis Using Advanced Data Science Methods Sunday, Nov 10, 3:30 PM

Hyatt Regency Orlando, Peacock Spring

Heather Mayes, Chair Xinrui Yu, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

3:30 Paper 38a: Deep Learning of Activation Energies and Automated Reaction Dataset Generation

— Colin A. Grambow, William H. Green

3:50 Paper 38b: Towards Automated Discovery of Plausible Reaction Paths in Complex Catalytic Systems Using Network Generation and Optimization — *Bowen Li, Srinivas Rangarajan, Ana*

4:10 Paper 38c: Robust Catalyst Characterization and Estimation of Mechanistic Pathways through Data Science

I. Torres

— M. Ross Kunz, Yixiao Wang, Rakesh Batchu, Zongtang Fang, Adam Yonge, Andrew Medford, Gregory S. Yablonsky, Rebecca Fushimi

4:30 Paper 38d: Autoneb: A Toolkit for Automating Reaction Network Calculation

— **Fang Liu**, Xiaolei Zhu, David Sanchez, Heather J. Kulik, Todd J. Martinez

4:50 Paper 38e: Recent Advances in Automated Transition State Theory Calculations: A Case Study Using Butanol

— **Nathan Harms**, Carl Underkoffler, Richard H. West

5:10 Paper **38f**: Smart Synthetic Path Generation System with Analysis of Reaction Risk Enhanced By Automated Open Data Collection

— **Joonsoo Jeong**, Dongil Peter Shin, Chang Won Kim, En Sup Yoon

5:30 Paper 38g: Reaction Network Analysis and Motifs for Rhythmic Dynamics in Metabolic and Circadian Models of Cyanobacteria in a Photobioreactor

— **Igor Schreiber**, František Muzika, Šafránek David, Jan Červený

(39) Reactor Engineering for Biomass Feedstocks

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Regency Ballroom T Yukihiko Matsumura, Chair

Paul Dauenhauer, Co-Chair Sponsored by: Sustainable Biorefineries

- **3:30 Paper 39a:** Supercritical Water Gasification of Shochu Residue in a 1 t/d Pilot Plant
- **Yukihiko Matsumura**, Shuhei Inoue, Takahito Inoue, Yoshifumi Kawai, Takashi Noguchi, Hiroaki Tanigawa
- **3:48** Paper **39b**: Alkyl Lactate Formation from the Depolymerization of Post-Consumer Polylactic Acid By Metal Complex Catalysts
- Luis Antonio Roman-Ramirez, Paul McKeown, Fabio Lamberti, Matthew Jones, **Joseph Wood**
- **4:06** Paper 39c: Kinetic Studies on the CO₂ Gasification of Biochar for Use with SOFCs As a Bioenergy with Carbon Capture and Sequestration (BECCS) Process
- Derek Ni, Amanda Simson
- **4:24** Paper 39d: Kinetic Modeling of the Thermal Decomposition of Pine Sawdust with the Dynamic Optimization Method
- **Andrew Seeger**, Hui Liu, Chandana Jayasooriya, Matthew Feeney
- **4:42 Paper 39e:** Heat and Mass Transfer during Torrefaction in the Packed Bed of Biomass
- **Ken-ichiro Tanoue**, Kentaro Hikasa, Akihiro Hideno, Miki Taniguchi, Ken-ichi Sasauchi
- **5:00** Paper 39f: The Production of Long Chain Hydrocarbons through the Catalytic Upgrade of Biomass-Based Acetone, Butanol and Ethanol (ABE)
- Elham Ketabchi, Laura Pastor-Perez, Tomás Ramirez-Reina, Harvey Arellano-Garcia
- **5:18** Paper 39g: Development and Economic Assessment of a Biphasic Process for 5-Hydroxymethylfurfural Production
- **Jonathan C. Overton**, Abigail S. Engelberth, Nathan S. Mosier
- **5:36 Paper 39h:** Scale-up of a Catalytic Membrane Reactor for the Production of 5-Hydroxymethylfurfural from Lignocellulosic Biomass
- **Tanmoy Patra**, Bob Beitle Jr., Richard J. Ciora, S. Ranil Wickramasinghe, Xianghong Qian
- (40) Self and Directed Assembly at the Nanoscale

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Discovery 45 Erick S. Vasquez, Chair Shohreh Hemmati, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

- **3:30 Paper 40a:** Nanowires through Oriented Attachment or Nanoscale Self-Assembly
- Younan Xia
- **3:55 Paper 40b:** Directed Assembly of Paramagnetic Colloids in Time-Varying Magnetic Fields
- Sibani Lisa Biswal

- **4:20 Paper 40c:** A New Class of Colloidal Gel Based on the Solvent Segregation Assisted Particle Self-Assembly
- Yuyin Xi, Yun Liu
- **4:36 Paper 40d:** Adsorption Dynamics of Polymeric Nanoparticles at an Air-Water Interface with the Addition of Surfactants
- **Chang Tian**, Jie Feng, Robert K. Prud'homme
- **4:52 Paper 40e:** Mechanisms of Nanoparticle Haloing for the Control of Colloidal Stability
- Marzieh Moradi, **Vance Jaeger**, Gerold A. Willing, Stuart J. Williams
- **5:08** Paper **40f**: Mechanistic Understanding of the Nanoparticle Self-Assembly By Coupling Inter-Particle Forces from Real-Time Measurements *Jaewon Lee*
- **5:24 Paper 40g:** Probing Nanocrystal Shape Transformations Using Parallel Tempering Molecular Dynamics and the Mold Method
- Tianyu Yan, Kristen Fichthorn
- **5:40** Paper **40h**: Self-Assembly of Nanoparticles at Membrane Interface *Amir H. Bahrami*, *Carol K. Hall*
- (41) Software Tools and Implementations for Process Systems Engineering

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Bayhill 26 Bethany Nicholson, Chair Benoit Chachuat, Co-Chair

Sponsored by: Computing Systems and Technology Division

- 3:30 Paper 41a: MAiNGO —
 McCormick-based Algorithm for MixedInteger Nonlinear Global Optimization
 Jaromił Najman, Dominik Bongartz,
 Susanne Sass, Jannik Burre, Hatim
 Djelassi, Wolfgang R. Huster, Kaan
 Karacasulu, Artur M. Schweidtmann,
 Alexander Mitsos
- **3:49** Paper **41b**: Graph-Based Abstractions and Tools for the Modeling and Simulation of Cyber-Physical Systems *Jordan Jalving*, *Yankai Cao*, *Victor M. Zayala*
- **4:08** Paper 41c: Industrial Modeling & Programming Language (IMPL): A Platform for Offline and Online Optimization and Estimation Applications
- **Jeffrey D. Kelly**, Brenno C. Menezes
- **4:27** Paper 41d: General Adsorbent Library and Evaluation (GALE) Software Tool for CO₂ Capture
- **Seongbin Ga**, Sangwon Lee, Jihan Kim, Jay H. Lee
- **4:46** Paper 41e: Chemsheet As a Simulation Platform for Modelling Industrial Concentrates and Brines Karri Penttilä, Risto Pajarre, Peter Blomberg, Marja Nappa, Petteri Kangas, Pertti Koukkari

- **5:05** Paper **41f**: Decode Automated Structure-Based Decomposition and Decomposition-Based Solution of Optimization Problems
- **Wentao Tang**, Ilias Mitrai, Andrew Allman, Prodromos Daoutidis
- **5:24** Paper 41g: Towards a Unified Strategy and Prototype Software Platform for the Synthesis of Operable & Sustainable Process Intensification Systems
- Yuhe Tian, Salih E. Demirel, Jianping Li, Styliani Avraamidou, Anjan Kumar Tula, Mario Richard Eden, **M. M.** Faruque Hasan, Rafiqul Gani, Efstratios N. Pistikopoulos
- **5:43** Paper 41h: A Toolbox for Integrated Process Design, Control and Analysis
- Anjan Tula, Jialiang Wang, Mario Richard Eden, Xi Chen, **Rafiqul Gani**
- (42) Solid Form Selection: Cocrystals, Salts, Solvates, Polymorphs, and Beyond

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Coral Spring I/II Xiaobin Jiang, Chair Gaurav Giri, Co-Chair

Sponsored by: Crystallization and Evaporation

- 3:30 Welcoming Remarks
- **3:33 Paper 42a:** Importance of Cocrystal Discovery Workflow for API Purification and Development
- **Samir Kulkarni**, Geoffrey Wood, Frank Pickard IV, Kris Jones, Brian P Chekal
- **3:51 Paper 42b:** Study on the Non-Isothermal Dehydration Kinetics of Cefminox Sodium
- **Suya Ma**, Baoshu Liu, Hua Sun
- **4:09** Paper **42c**: The Role of Crystallizability, Polymorphism and Drug Species in Drug Candidate Selection *Lotfi Derdour*
- **4:27 Paper 42d:** Spatial Confined Capillary Flow Involved Model for Micro Droplet Crystallization and Particle Screening
- Jin Li, Mingguang Han, Xiaobin Jiang, Gaohong He
- **4:45** Paper **42e**: A Combined Theoretical and Experimental Investigation into the High Throughput Screening of Cocrystal Coformers *Isaac J. Sugden, Claire S. Adjiman, Costas C. Pantelides, Doris Braun*
- **5:03** Paper **42f:** Insight into the Role of Pre-Assembly and Desolvation in Crystal Nucleation: A Case of p-Nitrobenzoic Acid **Shuyi Zong**, Hongxun Hao, Hao Wu, Qi Liu, Xin Huang
- **5:21** Paper **42g**: Utility of Phase Diagram Models in Crystallization Process Development the Case of an LLPS-Mediated Reactive Crystallization
- Venkateswarlu Bhamidi

- **5:39** Paper 42h: Surprising Effect of Carbon Chain Length on Inducing Ability of Additives: Elusive Form- of γ-Aminobutyric Acid (GABA) Induced By Sodium Carboxylate Additives

 Lingyu Wang, Weiwei Tang, Junbo
- 5:57 Concluding Remarks

(43) Value-Added Co-Products from Lignin for Biorefineries

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Regency Ballroom V

Rebecca Ong, Chair Justinus A. Satrio, Co-Chair

Sponsored by: Sustainable Biorefineries

- **3:30** Paper 43a: Fractionation and Purification of Biorefinery Lignins Using Aqueous Renewable Solvents

 Graham W. Tindall, Mark C. Thics.
- **Graham W. Tindall**, Mark C. Thies, David Hodge
- **3:55 Paper 43b:** Evaluating Endocarp Biomass As Potential Feedstocks for Biorefinery
- **Makua Vin-Nnajiofor**, Jian Shi, Seth Debolt
- **4:20 Paper 43c:** Lignin Fractionation for Quality Carbon Fiber
- **Qiang Li**, Cheng Hu, Mengjie Li, Joshua Yuan
- 4:45 Paper 43d: Sandbox (Hura crepitans) Oil Methyl Esters Synthesis: Process Modeling, Optimization, Kinetics and Thermodynamics Studies Jennifer C. Oraegbunam, Babatunde Oladipo, Olayomi A. Falowo, Eriola Betiku
- **5:10** Paper 43e: Computational Fluid Dynamics Simulation of Compressible Non-Newtonian Biomass in a Compression-Screw Feeder
- **Mohammad J. Rahimi**, Hariswaran Sitaraman, James J. Lischeske, David A. Sievers, Jonathan J. Stickel
- **5:35 Paper 43f:** Evaluation of Co-Pyrolysis of Lignin and Plastics through Thermogravimetric Analysis
- **Chang Dou**, Jie Chen, Sunkyu Park, Stephen S. Kelley

(44) Value-Added Uses of Industrial Coproducts in Sustainable Uses Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Discovery 47 Manju Misra, Chair Amar K. Mohanty, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

- **3:30 Paper 44a:** Kraft Lignin Color Reduction for Potential UV Absorbent Applications in Transparent and UV Protection Films
- **Mahesh Parit**, Zhihua Jiang
- **3:50** Break

4:10 Paper 44c: Multistream Integrated Biorefinery Achieved By Integration of Lignin Bioconversion and Carbon Fiber Manufacturing

— Cheng Hu

4:30 Paper 44d: Enhancing Fertility of Marginal Soils Using Lignin-Rich Hydrolysis Residues

— Meredith Grusnick, Sarvada Chipkar, Chris Miller, Martin Jurgensen, **Rebecca Ong**

4:50 Paper 44e: Evaluation of Pennycress Biochar for Adsorption of Nitrophenols from Water

— **Veera M. Boddu**, Sanghoon Kim, Steven C. Peterson, Ashley Maness, Manoj Shukla, Reddy Damavarapu

5:10 Paper 44f: Surface Tension Analysis of Lignin Nanoparticles and Cellulose Nanocrystals with Magnetic Properties in Water-Ethanol Mixtures Under Varying Experimental Conditions — Frankie A. Petrie, Grace Docken, Mary Worbington, Mohammad J. Hasan, Esteban E. Ureña-Benavides, Erick S. Vasquez

5:30 Paper **44g**: Enhanced Flame Retardancy of Poly(butylene terephthalate) with Biobased Flame Retardant

— Boon Peng Chang, Suman Thakur, Amar K. Mohanty, **Manju Misra**

(45) Vapor Phase Processing of Materials

Sunday, Nov 10, 3:30 PM Hyatt Regency Orlando, Celebration 15

Selma Mededovic Thagard, Chair Mahendra Sunkara, Co-Chair

Sponsored by: Electronics and Photonics

3:30 Paper 45a: Halide Vapor Phase Epitaxy of III-V Semiconductors on Silicon Substrates

— **Sonia Calero-barney**, Mahendra K. Sunkara

3:50 Break

4:10 Paper **45c**: Effect of Deposition Method on Valence Band Offsets of SiO₂ and Al₂O₃ on (Al_{0.14}Ga_{0.86})₂O₃

— **Chaker Fares**, Fan Ren, David C. Hayes, Brent P. Gila, Stephen J Pearton

4:30 Paper **45d**: Au-Pd Alloys for Near-Infrared Hot Carrier Devices: Structural, Electronic and Optical Properties

— **Kevin M. McPeak**, Sara K. F. Stofela, Orhan Kizilkaya, Tiago R. Leite, William A. Shelton Jr., Phillip T. Sprunger, Jason B. Baxter, Mohammad Mehdi Taheri

4:50 Paper **45e**: Scanning Electron Microscopy Measurements of the Luminescent and Electrical Properties of Thin Film Photovoltaic Devices

— Taylor B. Harvey, Aida Torabi

5:10 Paper 45f: High-Temperature, High-Pressure Molecular Doping of Nanodiamond for Sensing Applications — *Matthew Crane*, Alessio Petrone, Ryan Beck, Matthew Lim, Xuezhe Zhou, Xiaosong Li, Rhonda Stroud, Peter Pauzauskie

(46) Workshop: Effective Teaching for New or Prospective Faculty

Sunday, Nov 10, 3:30 PM
Hyatt Regency Orlando, Rock Spring I/II
Lisa G. Bullard, Chair
Donald P. Visco Jr., Co-Chair
David L. Silverstein, Co-Chair

Sponsored by: Professional Development Committee Liaison

3:55 Welcoming Remarks

4:00 Workshop

(47) Workshop: Writing Successful Education Proposals Sunday, Nov 10, 3:30 PM

Hyatt Regency Orlando, Bayhill 23
Milo D. Koretsky, Chair
Matthew Cooper, Co-Chair

Sponsored by: Education

3:30 Paper 47a: You Can Do It! Overcome Common Challenges in Engineering Education Research

- Matthew Cooper, Milo D. Koretsky

(48) Order of the Engineer Sunday, Nov 10, 5:00 PM Hyatt Regency Orlando, Plaza International Ballroom I

Sponsored by: Licensing and Professional Development Committee

(49) Agglomeration and Granulation Processes

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 20 Stephen L. Conway, Chair Brendon G. Ricart, Co-Chair

Sponsored by: Particle Production and Characterization

8:00 Paper 49a: Use of Bentonite Binder to Optimize Granulation Process during Fertilizer Manufacture

— Natsai Mushonga, **Nkosikhona Hlabangana**

8:21 Paper 49b: Compartmental Modelling of Wet Granulation in Twin Screw Using Population Balance

— **Hamza Ismail**, Mehakpreet Singh, Saeed Shirazian, Darren Whitaker, Ahmad B. Albadarin, Gavin Walker

8:42 Break

9:03 Paper 49d: Coagulation of Polydisperse Primary Particles in the Transition Regime

— Eirini Goudeli, Georgios A. Kelesidis

(50) Applications of Molecular Modeling to Study Interfacial Phenomena I

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Rock Spring I/II Harold W. Hatch, Chair Vance Jaeger, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

8:00 Paper 50a: Metal Decorated Graphene Catalysts for the ORR: Effects of Nanoparticle Size, Composition, and Support Dopant on Activity

— **Rees B. Rankin**, Tamara Lozano

8:15 Paper 50b: Assembly of Gold Nanowires on Gold Nanopad Arrays: Simulation and Experiment

— **Omid Jahanmahin**, David Kirby, Christine D. Keating, Kristen Fichthorn

8:30 Paper 50c: Role of Chloride in the Shape-Selective Growth of Ag Nanocrystals

- Zihao Chen, Kristen Fichthorn

8:45 Paper 50d: Using Enhanced Sampling Methods to Study the Behavior of Osteocalcin on Mineral Surfaces

— **Sarah Alamdari**, Rachel Gebhart, Gary Drobny, Jim Pfaendtner

9:00 Paper 50e: Adsorption and Disintegration of Surfactant Micelles at Metal-Water Interfaces: A Computational Investigation

— **Himanshu Singh**, Yathish Kurapati, Sumit Sharma

9:15 Paper 50f: Molecular Self-Assembly of Organometallic Complexes on 2D Materials: A Molecular Dynamics Study

- Hessam Malmir, Victor S. Batista

9:30 Paper 50g: A Molecular Dynamics Study to Investigate the Structural Features of Surfactant Aggregates Adsorbed at Mineral/Water Interfaces — Anuradha Bhat, Xiaoyu Wang, Sohail Murad, Michael T. Harris

9:45 Paper 50h: Fluid Transport in Shale Nanopores

- Tuan Ho, Yifeng Wang

10:00 Paper 247i: Thermodynamic Techniques to Capture Non-Ideal Surfactant Assembly at Hard Nanoscale Interfaces

— Junwoong Yoon**, Zachary Ulissi**

10:15 Paper 50j: Impacts of Entropic Separation Effects

- Alexander von Wedelstedt, Grit Kalies

(51) Big Data and Analytics for Sustainability

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Regency Ballroom T William M. Barrett, Chair Nastassja Lewinski, Co-Chair Raymond L. Smith, Co-Chair

Sponsored by: Sustainability Science and Engineering

8:00 Paper 51a: Sustainability in Saudi Aramco: Planning & Optimization

— *Mohammed Alyanbaawi*

8:25 Paper 51b: Applying Machine Learning to Estimate Releases from New Uses of Existing Chemicals

— Raymond L. Smith, Jose D. Hernandez-Betancur, David E. Meyer, Gerardo J. Ruiz-Mercado, William M. Barrett, Michael A. Gonzalez, John P. Abraham **8:50 Paper 51c:** Supply Chain Management of Livestock Waste for Spatio-Temporal Control of Nutrient Pollution in Water Bodies

— **Yicheng Hu**, Apoorva Sampat, Gerardo J. Ruiz-Mercado, Victor M. Zavala

9:15 Paper **51d:** Introducing a New Quantitative Life Cycle Assessment Module for Biofuels and Bioproducts — *Rui Shi, Yoel Cortes-Pena, Jeremy Guest*

9:40 Paper 51e: A Data-Driven Framework for Biomass Selection and Process Optimization of Activated Carbon Production

- Mochen Liao, Steve Kelley, Yuan Yao

10:05 Paper 51f: A Personal Exposure Agent Based Model (ABM) with the Capacity of Aggregation at Various Levels of Population Size

— Dimitrios Chapizanis, Spyros Karakitsios**, Dimosthenis Sarigiannis**

(52) Big Data and Data Analytics (Invited Talks)

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 27 Leo H. Chiang, Chair Mona Bavarian, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Introductory Remarks

8:10 Paper 52a: Data Science and Machine Learning in the Upstream Oil and Gas Industry

— Thomas Halsey

8:45 Paper 52b: Big Data Analytics in the Advanced Manufacturing of Biopharmaceuticals

— **Richard D. Braatz**, Weike Sun

9:20 Paper 52c: Big Data Impact on the Future of Manufacturing
— *Lisa Graham*

9:55 Paper 52d: Data-Assisted Modeling and Optimization for Process Systems Engineering

— Fani Boukouvala

(53) Biomaterials and Life Science Engineering: Faculty Candidates II

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 7 Mark W. Tibbitt, Chair Whitney L. Stoppel, Co-Chair Handan Acar, Co-Chair Audie Thompson, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 53a: Increasing the Dimensionality of Single Cell Transcriptomics to Address Systems Biology: Proteins, Imaging, and More — Alex Xu. James R. Heath

8:18 Paper 53b: Orchestrating Innate Immunity Against Cancer Using Nanotechnology

— Fan Zhang

- **8:36** Paper **53c:** Enhanced *In Vivo* Neuronal Survival after Traumatic Brain Injury Facilitated By an Injectable Self-Assembled Peptide Hydrogel
- **Biplab Sarkar**, Xiaotang Ma, Patricia Iglesias-Montoro, Zain Siddiqui, Agnieszka Agas, Ka Kyung Kim, James Haorah, Vivek Kumar
- **8:54 Paper 53d:** Living Composite Materials of Cells, Polymeric Scaffolds, and Artificial Proteins
- **Seunghyun Sim**, David A. Tirrell
- **9:12** Paper **53e:** Single Molecule Study of Charge Transport in Redox Active Biomolecules
- **Bo Li**, Songsong Li, Andrew D. Ellington, Eric Anslyn, Charles M. Schroeder
- **9:30 Paper 53f:** Engineered Nanomaterials Enable Transgene-Free Plant Genetic Transformations
- **Gozde Sultan Demirer**, Huan Zhang, Juliana Matos, Natalie Goh, Francis Cunningham, Younghun Sung, Brian Staskawicz, Markita Landry
- **9:48** Paper **53**g: Multi-Scale Dynamics of Biological Systems and Active Matter *Brad A. Krajina*
- 10:06 Paper 53h: Investigating
 Molecular Interactions of the Placenta
 for Prenatal Treatment and Testing
 Christina Bailey-Hytholt, Anubhav
 Tripathi, Anita Shukla

(54) Biomaterials from Lignocellulosics

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Discovery 47

Justinus A. Satrio, Chair Shijie Liu, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

- **8:00** Paper 54a: Efficient Conversion of Pulp and Paper Sludge to Cellulose Nanomaterials and Their Application As Building Blocks for Constructing Conductive Nanopapers and Hydrogels Haishun Du, Mahesh Parit, Zhihua Jiang, Bin Li, Xinyu Zhang
- **8:25** Paper 54b: Rheological Characterization of Nanocellulose Materials for Quality Control
- **Jianshan Liao**, Kim Anh Pham, Victor Breedveld
- **8:50 Paper 54c:** Cellulose Nanofiber and Polypyrrole Based Conducting Composite Films with Improved Conductivity, Strength, Water Resistance and Electromagnetic Shielding Properties
- **Mahesh Parit**, Haishun Du, Xinyu Zhang, Zhihua Jiang
- **9:15** Paper **54d:** Immobilization of Antibodies on Cellulose Nanocrystals for the Detection of Cancer Biomarkers
- **Uma Madhuri Nori**, Diego Gómez Maldonado, Partha Saha, Maria Soledad Peresin, Virginia Davis

- **9:40 Paper 54e:** High Shear Behavior of Nanocellulosics
- **Michael J. Bortner**, Jeffrey Youngblood, Bradley Sutliff

(55) Biomimetic Materials II Monday, Nov 11, 8:00 AM

Hyatt Regency Orlando, Celebration 5 R. Helen Zha, Chair Neha Kamat, Co-Chair Marjan Rafat, Co-Chair Xi Chen, Co-Chair

Sponsored by: Biomaterials

- **8:00 Paper 55a:** Development of a Model Placental Lipid Bilayer
- **Christina Bailey-Hytholt**, Tun-Li Shen, Anubhav Tripathi, Anita Shukla
- **8:18** Paper 55b: A Particle-Based Network Biomimetic Material System for Assay and Spectroscopy of Membrane Proteins in Intact Lipid Bilayers

 M. Lane Gilchrist, Robert J.
- **8:36 Paper 55c:** Engineering Selective Biomolecular Transport in Nucleoporin-

Messinger

- like Protein Hydrogels

 Danielle J. Mai, Yun Jung Yang,
 Bradley D. Olsen
- **8:54** Paper **55d:** Recent Advances in Mussel-Inspired Wet Adhesion *Kollbe Ahn*
- **9:12 Paper 55e:** Bioinspired Elastin-Based Protein Adhesives
- Sydney Hollingshead, Charng-yu Lin, Jonathan J. Wilker, **Julie C. Liu**
- **9:30 Paper 55f:** Bacterially Super Anti-Adhesive, Optically Transparent Coatings Inspired from Rice Leaves
- **Shuhao Liu**, Michael Bae, Jun Kyun Oh, Mustafa Akbulut
- **9:48** Paper **55g:** Collagen Thin Film Adhesion and Morphology Mediated By Siderophore Inspired Molecules
- Roberto C Andresen Eguiluz,
 George Degen, Garrett Lindsey, Eric
 Valois, Alison Butler

10:06 Paper **55h:** Mimicking Complex Morphologies of Calcium Biominerals — *Gopichand Mallam, Marina Tsianou*

(56) Biomolecules at Interfaces II Monday, Nov 11, 8:00 AM

Hyatt Regency Orlando, Plaza International Ballroom K Peter J. Beltramo, Chair Yeongseon Jang, Co-Chair Erick S. Vasquez, Co-Chair

Sponsored by: Interfacial Phenomena

- **8:00 Paper 56a:** Biosurfactants in Aqueous Solution: Self-Assembly and Surface Adsorption
- Yi Zhang, Paschalis Alexandridis, **Marina Tsianou**
- **8:17** Paper **56b:** Synthesis of Novel Fluorescent Surfactants and Their Interaction with Living Cells
- Shuai Kong, Chong Shen, Qin Meng
- **8:34** Paper **56c:** Assembly Dynamics of Bacterial Pore Forming Toxins on Lipid Membranes
- Rahul Roy

- **8:51 Paper 56d:** Protein and Lipid Sorting on the Bacterial Membrane Regulate Bacterial Outer Membrane Heterogeneity
- Justin Nice, Angela C. Brown
- 9:08 Paper 56e: Rheology of the Tear Film Lipid Layer in Health and Disease — Silvia Jonguitud-Flores, Rodrigo Velez-Cordero, Gabriel Espinosa-Pérez, Bernardo Yanez Soto
- **9:25 Paper 56f:** Effect of Dilatational Modulus on Lung Surfactant Functionality
- **Sourav Barman**, Joesph A. Zasadzinski
- 9:42 Paper 56g: Alpha-Synuclein-Mediated Membrane Remodeling — Brandon Hoover, Zhizhang Shen, Curran Gahan, Reid C. Van Lehn, Regina M. Murphy
- **9:59** Break
- **10:16** Paper **56i**: On the Collective Nature of Viral Protein Assembly and Membrane Lipid Reorganization during HIV-1 Budding
- Alexander J. Pak, Gregory A. Voth

(57) Carbon Dioxide Capture Technologies and Their Use

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Rainbow

Spring I/II
Sunil Hangal, Chair
Ángel Galán Martín, Co-Chair

Sponsored by: Climate Change

- **8:00 Paper 57a:** Solubility and Diffusivity of Syngas Components in a Next Generation Pre-Combustion Solvent
- **Lei Hong**, Nicholas Siefert, Robert Thompson, Wei Shi, Kevin P. Resnik, David Hopkinson
- **8:19** Paper **57b**: Carbon Capture and Storage (CCS): The Way Forward *Mai Bui*, *Niall Mac Dowell*
- **8:38 Paper 57c:** Corrosion Analysis of RTI's Non-Aqueous Solvent for Carbon Capture
- **Paul Mobley**, Aravind V. Rayer, Jak Tanthana, Vijay Gupta, Mustapha Soukri, Marty Lail, S. James Zhou
- **8:57 Paper 57d:** Catalytic Oxygen Removal from Pressurized Oxy-Combustion Flue Gases Using a Reverse Flow Fixed-Bed Reactor
- **Hong Lu**, Abiodun Oki, Luke Schideman, Yongqi Lu
- **9:16 Paper 57e:** Optimal Techno-Economic Design and Operation of a Fixed Bed System Using Micro-Encapsulated Solvent for CO₂ Capture
- **Goutham Kotamreddy**, Ryan Hughes, Debangsu Bhattacharyya, Joshua K. Stolaroff, Benjamin P. Omell, Michael S. Matuszewski
- **9:35 Paper 57f:** Techno-Economic Analysis of Post-Combustion Carbon Capture with a 3rd Generation Water-Lean Solvent
- Yuan Jiang, Paul M. Mathias, Greg Whyatt, Charles J. Freeman, Richard Zheng, David J. Heldebrant

(58) Catalysis with Microporous and Mesoporous Materials I: Gas-Phase Reactions

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Florida Ballroom A

Michele L. Sarazen, Chair David Hibbitts, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00 Paper 58a:** Hierarchical Gallosilicate MFI Catalyst Development for Natural Gas Conversion
- **Yuxin Wang**, Qingyuan Li, Xinwei Bai, Brandon Robinson, Ashley Caiola, Amoolya Lalsare, Jianli Hu
- **8:20** Paper 58b: Selective Production of Aromatics By Catalytic Fast Pyrolysis of Furan with in-Situ Dehydrogenation of Propane
- Xiaoduo Qi, Wei Fan
- **8:40 Paper 58c:** Evolution of Coke in a Fluid Catalytic Cracking Process
- Qandeel Almas, Awais Naeem, Christoph Muller, Jeffery Kenvin, Christopher Jones, Carsten Sievers
- **9:00** Paper 58d: Analysis of Kinetic and Diffusive Restraints on Methylbenzene Interconversion Pathways during MTO Using DFT and Kinetic Monte Carlo Simulations

 Mykela DeLuca, David Hibbitts
- **9:20** Paper 58e: Toluene Alkylation with Methanol in Brønsted Acid Zeolites *Taha Salavati-fard*, Deependra Parmar, Jeffrey D. Rimer, Lars C. Grabow
- **9:40** Paper 58f: Mechanistic Insight into Ethene Oligomerization over H-MFI *Danna Nozik*, *Erum Mansoor*, *Alexis T Roll*
- **10:00 Paper 58g:** Improving Long Chain Hydrocarbon Formation in Dimethyl Ether Homologation over Mesoporous Hbea Supported Cu Catalysts
- Anh To

(59) Charged and Ion-Containing Polymers I

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 11 Samanvaya Srivastava, Chair Vivek Sharma, Co-Chair

Sponsored by: Polymers

- **8:00** Paper 59a: Time-Temperature and Time-Water Superposition Principles Applied to Poly(allylamine) / Poly(acrylic acid) Complexes
- **Jodie L. Lutkenhaus**, Maria Sammalkorpi, Pilar Suarez Martinez, Piotr Batys
- 8:12 Paper 59b: Structure and Dynamics of Polyelectrolyte Complexes in Solid-to-Liquid Phase Transition
 Siqi Meng, Jeffrey M. Ting, Hao Wu, Matthew V. Tirrell

- **8:24** Paper **59c**: Dynamics of Entangled Liquid Coacervates Made from Oppositely Charged Polyelectrolytes
- **Christian Aponte-Rivera**, Michael Rubinstein
- **8:36** Paper 59d: Salt- and pH-Induced Swelling Behavior of a Poly(Acrylic acid) Brush Via Quartz Crystal Microbalance w/ Dissipation (QCM-D)
- **Nisha Hollingsworth**, Sabina Wilkanowicz, Ronald G. Larson
- **8:48** Paper **59e**: Pinch-Off Dynamics, Extensional Rheology and Printability of Polyelectrolyte Solutions
- **Leidy N. Jimenez**, Jelena Dinic, Vivek Sharma
- **9:00 Paper 59f:** Model of Equilibrium over-Charging in Polyelectrolyte Complexes
- Mohsen Ghasemi, Ronald G. Larson
- **9:12** Paper **59g**: Tunable Coacervation from Stoichiometrically Asymmetric Homologous Polyions
- Sean Friedowitz, Jian Qin
- **9:24 Paper 59h:** Complex Coacervates of Semiflexible Polyanions and Flexible Polycations: Isotropic and Liquid-Crystalline States
- Artem Rumyantsev, Juan de Pablo
- **9:36 Paper 59i:** Charge Sequence and Assembly in Polyelectrolyte Complex Coacervates
- Tyler Lytle, Gary Ong, Li-Wei Chang, Sarah L. Perry, **Charles E. Sing**
- 9:48 Paper 59j: Engineering
 Polyelectrolyte and Protein
 Complexation and Phase Separation
 Allie Obermeyer, Nicholas
 Zervoudis, Rachel Kapelner, Justin Horn
- **10:00 Paper 59k:** Evaluating Physical Properties and Stability of Nucleic Acid Polyelectrolyte Micelles
- **Alexander E. Marras**, Jeffrey Vieregg, Jeffrey M. Ting, Matthew V. Tirrell
- **10:12** Paper **59I**: A Materials Genome Approach to Unravel the Formation, Growth, and Demise of Complex Coacervate Assemblies
- **Jeffrey M. Ting**, Hao Wu, Siqi Meng, Abraham Herzog-Arbeitman, Matthew V. Tirrell

(60) Combustion Kinetics and Emissions

Monday, Nov 11, 8:00 AM
Hyatt Regency Orlando, Plaza
International Ballroom F
Bihter Padak, Chair
Richard H. West, Co-Chair
C. Franklin Goldsmith, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 60a: Autonomous Systems for Experimental and Data-Driven Modeling of Combustion Kinetics

— Sai Krishna Sirumalla, Nathan

— Sai Krishna Sirumalla, Nathan Harms, Mark Barbet, Carly LaGrotta, Michael Burke, Kyle Niemeyer, Richard H. West

- **8:19** Paper 60b: Ash Formation in Co-Firing Torrefied Wood with Coal on a Pilot-Scale Air/Oxy-Fuel Combustor
- **Xiaolong Li**, Yueming Wang, Jianqun Wu, Minghou Xu, Dunxi Yu, Jost O. L. Wendt
- **8:38** Paper 60c: Effects of Fluidizing Gas on Copper-Manganese Mixed Oxide's Reactivity for Chemical Looping Combustion of CH,
- Turna Barua, Bihter Padak
- **8:57 Paper 60d:** Ash Partitioning and Deposition Mechanisms in Rice Husk Combustion
- **Yueming Wang**, Jianqun Wu, Xiaolong Li, Jingkun Han, Minghou Xu, Dunxi Yu, Jost O. L. Wendt
- **9:16 Paper 60e:** Sustained Oscillations Caused By Feed Modulation during Methane Oxidation on Four-Way Catalysts
- **Kyle Karinshak**, Steve Golden, Michael Harold
- **9:35 Paper 60f:** Deconvoluting Transient Water Effects on the Activity of Pd Methane Combustion Catalysts
- Weixin Huang, Emmett Goodman, Matteo Cargnello
- **9:54** Paper **60g**: Global Reaction Kinetics in Commercial Three-Way Catalysts (TWCs)— an Experimental and Modeling Study
- **Ritesh P. Mohanty**, Hrushikesh Pimpalgaonkar, Natarajan Gunasekaran, Kunal Sakekar, David R. Heine
- **10:13 Paper 60h:** Effects of Preparation Parameters on Simultaneous Removal of Hg(0) and NO over Modified SCR Catalyst
- Can Li, Joo-Youp Lee

(61) Free Forum on Engineering Education: First Year and Sophomore Year

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 23 Sandra L. Pettit, Chair Katie Cadwell, Co-Chair

Sponsored by: Undergraduate Education

- **8:00 Paper 61a:** Flow Chemistry Case Study for Material and Energy Balance Course
- Laura Jarboe
- **8:21 Paper 61b:** A Summer Overseas Experience at the Imperial College CO₂ Capture Pilot Plant
- Mark J. McCready
- **8:42** Paper 61c: Design Challenges As a Spine to Chemical Engineering Courses
- **Abhaya K. Datye**, Jamie Gomez, Marina Miletic, Eva Y. Chi, Sang M Han, Catherine Hubka, Yan Chen, Vanessa Svihla, Pil Kang
- **9:03 Paper 61e:** Development of the Chemical Engineering Identity from the Freshman to the Sophomore Year
 - Gerold A. Willing

- **9:24** Paper 61f: Can Enriched Extracurricular Activities Influence Early Undergraduate Students' Interest and Participation in Chemical Engineering Design Teams?
- Sindia Rivera-Jimenez
- **9:45 Paper 61g:** Measuring Spreadsheet Skills Using Analytics within an Interactive Textbook
- Matthew Liberatore
- 10:06 Paper 61h: Retention Improvement Efforts in the Undergraduate Living and Learning Community at the University of South Carolina
- Edward P. Gatzke

(62) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains I

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Regency Ballroom V

Dharik Mallapragada, Chair Fengqi You, Co-Chair Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by: Sustainable Energy

- **8:00 Paper 62a:** Supply Network Optimization of Carbon Capture, Sequestration and Utilization from Point Sources
- **Tina Kegl**, Lidija Čuček, Anita Kovač Kralj, Zdravko Kravanja
- **8:25 Paper 62b:** Large Scale Deployment of Low Carbon Hydrogen and CCS Value Chains for the Decarbonisation of Heat: Novel Methods and Insights
- **Nixon Sunny**, Niall Mac Dowell, Nilay Shah
- **8:50 Paper 62c:** Cost-Effectiveness of Continuous H₂ Production Using Integrated PV-Electrolysis-Storage Systems
- **Dharik Mallapragada**, Patrick Insinger, Emre Gençer
- **9:15** Paper **62d**: Economic Analysis of Integrated Solar Power, Hydrogen Production, and Electricity Markets
- Omar J. Guerra, Mariya N. Koleva, Joshua Eichman, Jennifer Kurtz, Bri-Mathias Hodge
- **9:40 Paper 62e:** Simultaneous Design and Operation of Renewable Energy Carrier Production
- **C. Doga Demirhan**, William W. Tso, Clara F. Heuberger, Joseph B. Powell, Efstratios N. Pistikopoulos

(63) Development of Intermolecular Potential Models

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Silver Spring

Neeraj Rai, Chair Nav Nidhi Rajput, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **8:00** Paper 63a: Experimental Validation of 2- and 3-Body Ab Initio Potentials for Helium-4 Via Second to Seventh Virial Coefficients
- **Navneeth Gokul**, Andrew J. Schultz, David A. Kofke
- **8:17 Paper 63b:** Relative Resolution: Implementation in Lammps for Organic Systems
- Aviel Chaimovich
- **8:34** Paper 63c: Assessment of Molecular Dynamics Force Fields for Conjugated Polymers Using Neutron and X-Ray Scattering
- Caitlyn Wolf, Lilo Pozzo
- **8:51 Paper 63d:** Automation of Non-Bonded Parameter Optimization in Molecular Mechanics Force Fields
- **Mohammad Barhaghi**, Younes Nejahi, Richard A. Messerly, Loren Schwiebert, Jeffrey J. Potoff
- **9:08** Paper 63e: The Open Force Field Initiative: Better Force Fields through Open, Data-Driven Science
- Michael R. Shirts, David L. Mobley, John Chodera, Lee-Ping Wang, Michael K. Gilson
- **9:25** Paper 63f: Theoretical Phase Diagram of Self-Assembled Patchy Particles: Fluid and Solid Phases *Yiwei Zhu, Walter G. Chapman*
- **9:42 Paper 63g:** A Simulation Database for Applications of Mbar to Force Field Development
- **S. Mostafa Razavi**, J. Richard Elliott Jr.
- **9:59 Paper 63h:** Anomalies in Supercooled Water at ~230 K Arise from Topological Transformation
- **Saber Naserifar**, William A. Goddard III
- **10:16** Paper **63i**: Atomistic Force Field Model Development for the Thiolate/ Defective Au (111) Interface
- **Guobing Zhou**, Liangliang Huang, Lloyd A. Bumm

(64) Developments in Catalytic Conversion to Chemicals

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Challenger 38/39

Sheima J. Khatib, Chair Hilal Ezgi Toraman, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

- **8:00** Paper 64a: Oxidative Coupling Methane Enhanced By Distribution of Oxygen through Porous Medium *Geo-Jong Kim*, *Hyun-Tae Hwang*
- **8:21 Paper 64b:** Direct Conversion of Methane to Aromatics Using Metal
- Raj Thakur, Carlos Carrero

Carbides

- **8:42** Paper 64c: Fe_O_3@SBA-15 As an Efficient and Stable Catalytic Oxygen Carriers for Chemical Looping Partial Oxidation of Methane to Generate Syngas
- **Yan Liu**, Lang Qin, Zhuo Cheng, Josh Goetze, Liang-Shih Fan

9:03 Paper 64d: The Effect of Reducing Agents (H₂, CO and Syngas) on Cobalt-Based Catalysts for Fischer Tropsch Synthesis

- Nothando Shiba

9:24 Paper 64e: Stability of Supported Metal Oxide Catalysts for the Non-Oxidative Dehydrogenation of Propane: An in Situ/Operando Raman Study - Rafael Sanchez, Jorge Moncada,

Carlos A. Carrero

9:45 Paper 64f: Investigation of Chabazite and Other Small-Pore Zeolites in the DME Carbonylation Reaction

- Marcella Lusardi. Mark E. Davis

10:06 Paper 64g: Competitive Transient Electrostatic Adsorption Mechanism for in Situ Regeneration of Poisoned Catalyst

— Yanbo Pan, Xiaochen Shen, Libo Yao, Abdulaziz Bentalib, Zhenmeng Peng

(65) Diagnostics, Treatments and **Theranostics**

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 12/13

Joshua D. Ramsey, Chair Yunshan Wang, Co-Chair

Sponsored by: Chemical Engineers in

8:00 Paper 65a: Self-Assembling Nanotechnology for Cancer Theranostics: From Computer-Assisted Design to In Vivo Applications

- Erik Laurini, Domenico Marson, Suzana Aulic, Maurizio Fermeglia, Sabrina Pricl

8:18 Paper 65b: Point-of-Care Sepsis Diagnostics

— **Jouha Min**, Ralph Weissleder, Hakho Lee, Fillip Swirski

8:36 Paper 65c: Magnetic Blood Purification for Pathogen and Circulating Tumor Cell Removal

— Inge K. Herrmann

8:54 Paper 65d: Design and **Development of Inorganic Nanoparticles** for Radioenhancement Therapy

- Lukas R. H. Gerken, Kerda Keevend, Anna L. Neuer, Inge K. Herrmann

9:12 Paper 65e: PSMA-Targeted Glucose Oxidase Nanoparticles for Directed Cytotoxicity Toward Prostate Cancer Cells

— Nicholas Flynn**, Joshua D. Ramsey**

9:30 Paper 65f: Hydrogel-Crosslinking By Minimally Invasive Surgical Modalities

— Tasmia Tasnim, Huanan Zhana

9:48 Paper 65g: Micromotors for Active **Drug Delivery in Gastrointestinal Tract** — Jinxing Li

10:06 Paper 65h: Inflammation Targeted Intravenous Dendrimer-Drug Therapy for Age Related Macular Degeneration

– Rangaramanujam Kannan

(66) Division Plenary: CAST (Invited Talks)

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Regency Ballroom O

Christos T. Maravelias, Chair **Prodromos Daoutidis, Co-Chair**

Sponsored by: Computing Systems and Technology Division

8:00 Paper 66a: Overview of CAST **Activities and Programming**

- Christos T. Maravelias, Prodromos **Daoutidis**

8:15 Paper 66b: Bounds for Multistage Stochastic Programs Under Endogenous Uncertainties

- **Zuo Zeng**, Selen Cremaschi

8:42 Paper 66c: Hybrid Mechanistic Data-Driven Modelling for Real-Time Dynamic Optimization of Large-Scale Rectification Systems: Application to Air Separation Units

Pascal Schäfer, Adrian Caspari, Adel Mhamdi, Alexander Mitsos

9:09 Paper 66d: Decomposing Optimization-Based Bounds Tightening Problems Via Graph Partitioning

- Michael Bynum, Anya Castillo Bernard Knueven, John D. Siirola, Carl D. Laird

9:36 Paper 66e: Existence and Properties of Multiple Steady States to Horizontal Ribbon Growth

- **Eyan Noronha**, B. Erik Ydstie

10:03 Paper 66f: A Quantitative Approach for Optimization of Alarm Identification and Rationalization

 Joshiba Ariamuthu Venkidasalapathy, Costas Kravaris, M. Sam Mannan

(67) Division Plenary: Chemical **Engineering Principles for** Nanotechnology (Invited Talks)

Monday, Nov 11, 8:30 AM Hyatt Regency Orlando, Discovery 45 Samantha A. Meenach, Chair Reginald E. Rogers Jr., Co-Chair

Sponsored by: Nanoscale Science and **Engineering Forum**

8:30 Paper 67a: Interactions of Engineered Nanomaterials with the Cell Plasma Membrane

- Amir M. Farnoud

9:30 Paper 67b: Shape-Selective Growth of Nanoscale Materials: Insights from Multi-Scale Theory and Simulation

- Kristen Fichthorn

(68) Division Plenary: Chemical **Engineering Roles in U.S. Department of Energy Environmental Management and Waste Cleanup Programs**

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Challenger 41/42

Thong Hang, Chair Debalina Sengupta, Co-Chair

Sponsored by: Nuclear Engineering Division

8:00 Paper 68a: Keynote Presentation - Monica C. Regalbuto

(69) Division Plenary: Gerhold and **Kunesh Awards on Separations** (Invited Talks)

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Manatee Spring II Marcus Mello, Chair

Roger D. Whitley, Co-Chair

Sponsored by: Separations Division

8:00 Paper 69a: Water Treatment and Desalination: from High Performance Membranes to Flexible Self-Adaptive Systems

- Yoram Cohen

8:25 Paper 69b: Manufacturing Fit-for-Purpose Membranes from Nanostructured Polymers

– William A. Phillip

8:50 Paper 69c: Control of Polymorphism and Crystal Size Distribution and in Pharmaceutical Crystallization

- Richard Braatz

9:15 Paper 69d: Carbon Nanotube Membranes for Separation of Fuels from Water

Rob McGinnis

9:40 Paper 69e: Manufacturing **Advanced Structured Contactors** with Integrated Heat Management Capabilities

- Ryan Lively

10:05 Paper 69f: Wind-Powered Ammonia Synthesis

- Edward L. Cussler, Deepak Ojha, Alon V. McCormick, Michael Reese

(70) Efficient Biological Processing of **Lignin to Bioproducts and Biofuels**

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Regency Ballroom Q

Bin Yang, Chair Arthur J. Ragauskas, Co-Chair Ning Sun, Co-Chair Joshua Yuan, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable **Energy and Environment**

8:00 Paper 70a: Strategies for Assessing and Improving Microbial **Utilization of Lignin-Derived Monomers**

- Kirsten Davis, Marge Rover, Davinia Salvachua, Ryan G. Smith, Gregg T. Beckham, Zhiyou Wen, Robert C. Brown, Laura Jarboe

8:21 Paper 70b: Developing Bacterial Pelletized Culture to Enhance Yield and Simplify Harvest for Lignin Bioconversion

- Bing Xu, Zhihua Liu, Furong Lin, Joshua Yuan

8:42 Paper 70c: Unlocking the Genetic Potential of Rhodopseudomonas Palustris CGA₀₀₉ for Lignin Valorization – Cheryl Immethun, Taity Changa, Rajib Saha

9:03 Paper 70d: Improving Resistance of Hyperthermophilic Laccase to Ionic Liquids for in Situ Lignin Valorization - Joseph Stevens, Jameson Hunter, Claire Dumon, David Rodgers, Jian Shi

9:24 Paper 70e: Computational Pathway Design for Funneling Lignin Intermediates to Aromatic Products — **Lin Wang**, Costas D. Maranas

9:45 Paper 70f: Enhancement of Polyhydroxyalkanoate Production By Co-Feeding Lignin Derivatives with Glycerol in Pseudomonas Putida KT₂₄₄₀ — Zhangyang Xu, Xiaolu Li, Naijia Hao,

Arthur J. Ragauskas, Bin Yang

10:06 Paper 70g: Conversion of Lignin into Biodegradable Plastic By Rhodopseudomonas Palustris - Brandi Brown, Mark R. Wilkins, Rajib Saha

(71) Electrochemistry for Applications in Sustainability

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom I Lauren F. Greenlee, Chair Karthish Manthiram, Co-Chair **Shelby Foster, Co-Chair** Linsey Seitz, Co-Chair

Sponsored by: Electrochemical Fundamentals

Holewinski

8:00 Paper 71a: Insights into the Electrochemical Conversion of Biomass Derivatives to Fuels and Chemicals – Alex Roman, Joseph Hasse**, Adam**

8:30 Paper 71b: Speeding up Electrochemical Separations with Energy Impunity Using Ionomer Binder Resin-Wafers

— Varada Menon Palakkal, Lauren Valentino, Qi Lei, Matthew Jordan, Yupo J. Lin, Christopher G. Arges

9:00 Paper 71c: Effect of Mass Transfer on the Electrochemical Oxidation of Carboxylic Acids on Boron Doped Diamond Electrodes

- Anke Arts, Thijs de Groot, Riaan Schmuhl, J. van der Schaaf

9:20 Paper 71d: Efficient Continuous **Electrokinetic Dewatering of Phosphatic** Clay Suspensions

Arthur Dizon, Mark E. Orazem

9:40 Paper 71e: Surface Modification of Pd Nanocube By Cu UPD for **Electrochemical Nitrate Reduction** Marta Hatzell, Seung Woo Lee, JeongHoon Lim, Jinho Park

10:00 Paper 71f: Probing Mechanisms of Electrochemical Sulfur Oxidation in Wastewater and Crude Oil

- William A. Tarpeh

10:20 Paper 71g: Flow Battery Electroanalysis:Electron-Transfer Kinetics of Aqueous Fe(III/II) at Noble Metal and Carbon Flectrodes

- Tejal Sawant, James R. McKone

10:40 Paper 71h: A Kinetic Model for Redox Active Organic Cycling

— **Benjamin Silcox**, Jing Jing Zhang, Ilya Shkrob, Lu Zhang, Levi T. Thompson

(72) Engineering in Cancer Biology and Therapy II: Mechanisms of Disease

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 2 Ebong Eno, Chair Shreyas Rao, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 72a: Investigating Matrix Stiffness Mediated Dormancy in Brain Metastatic Breast Cancer Cells Using a Hyaluronic Acid Hydrogel Platform — Akshay Narkhede, James Crenshaw, Shreyas Rao

8:18 Paper 72b: Fluid Shear Stress Causes Resistance to Chemotherapy Drugs in Breast Cancer

Ursula Triantafillu, Spenser Brown, Yonghyun (John) Kim

8:36 Paper 72c: Disturbed Flow Induced Endothelial Glycocalyx Degradation Promotes Cancer Cell Attachment to the Endothelium

— **Solomon Mensah**, Alina Nersesyan, Ian Harding, Mark Niedre, Vladimir Torchilin, Eno E. Ebong

8:54 Paper **72d**: Irradiated Extracellular Matrix Hydrogels Enhance Tumor Cell Proliferation and Invasion

— **Tian Zhu**, Steven M. Alves, Anastasia Shostak, Ninna Rossen, Marjan Rafat

9:12 Paper 72e: Physical Intimacy of Glioblastoma Cells with Astrocytes Elicits Metabolic Reprogramming of Glioma Cells

— **Kimberly M Stank**e, Christina Wilson, Oleh Khalimonchuk, Srivatsan Kidambi

9:30 Paper 72f: Myosin 1B Regulates the Extravasation of Brain-Targeting Cells and Shifts Metastatic Organ Targeting in Larval Zebrafish — Colin D. Paul. Kevin Bishop. Lisa M.

 Colin D. Paul, Kevin Bishop, Lisa N Miller Jenkins, Raman Sood, Kandice Tanner

9:48 Paper 72g: Activation of IRE,α By Palmitate Leads to Loss of Desmoplakin in Liver and Breast Cancer Cells

— Amrita Oak, Aritro Nath, Grace

10:06 Paper 72h: Evaluating the Role of Endothelial to Mesenchymal Transition in Breast Cancer Extravasation into the Brain — Pedram Motallebnejad, Samira M. Azarin

(73) Faculty Candidates in CoMSEF/ Area 1a

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Peacock Spring

Amir Haji-Akbari, Chair Jeremy C. Palmer, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 73a: Multiscale Electronic Coarse-Graining of Soft Materials Via Supervised Machine Learning

— **Nicholas Jackson**, Juan de Pablo

8:17 Paper 73b: Molecular Simulations and Machine Learning for Multicomponent Adsorption

— **Tyler R. Josephson**, Yangzesheng Sun, J. Ilja Siepmann

8:34 Paper 73c: Designing the Phase Behavior and Microstructure of Nanocrystal Linker Gels

— **Michael P. Howard**, Ryan B. Jadrich, Beth A. Lindquist, Delia J. Milliron, Thomas M. Truskett

8:51 Paper 73d: Multiscale Modeling and Enhanced Sampling to Examine Self-Assembly in Peptide and Peptoid Systems

- Janani Sampath, Jim Pfaendtner

9:08 Paper 73e: Modeling Thermodynamics and Kinetics at 2D Material Interfaces: Applications in Synthesis, Nanopore Formation, Wetting, and Catalysis

— **Ananth Govind Rajan**, Michael Strano, Daniel Blankschtein, Emily A. Carter

9:25 Paper 73f: Studying Inhomogeneous Ion-Containing Complex Fluids Using Polarizable Field-Theoretic Simulations

— **Douglas Grzetic**, Kris Delaney, Glenn H. Fredrickson

9:42 Paper 73g: The Role of Deformability in Determining the Structural and Mechanical Properties of Bubbles and Emulsions

— Arman Boromand

9:59 Paper 73h: Unraveling the Quantum Mechanical Catalytic Action of Methyltransferases with GPU-Accelerated Large-Scale Electronic Structure

— **Zhongyue Yang**, Fang Liu, Heather J. Kulik

10:16 Paper 73i: Molecular Simulations of Biomimetic Assembly

- Aviel Chaimovich

(74) Forum Plenary: Opportunities and Challenges with Journey from Industry 4.0 to Pharma 4.0

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 6 Moiz Diwan, Chair Shujauddin M. Changi, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 74a: Artificial Intelligence for Pharma 4.0: Challenges and Opportunities

- Venkat Venkatasubramanian

8:37 Paper 74b: Positioning for a Sustainable Future – Continuous Processing, Automation and Predictive Modeling for Efficient Biopharmaceutical Process Development and Manufacturing

- Shailendra Bordawekar

9:14 Paper 74c: Systems-Based Pharmaceutics – an End-of-Decade Report — *Costas Pantelides*, *Sean Bermingham*

9:51 Paper 74d: What Challenges Need to be Addressed, and What New Technological Approaches Are Needed to Put Life Sciences on Path to Pharma 4.0?

- Cathal Strain

(75) Fundamentals and Applications of Flow Assurance

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Challenger 40 Francisco Vargas, Chair Nagu Daraboina, Co-Chair

Sponsored by: Upstream Engineering and Flow Assurance Forum

8:00 Paper 75a: Experimental Characterization of Surfactant Application in Gas Wells and in Presence of Water and Condensates

— **Amita Kosambi**, Hamidreza Karami, Sepideh Razavi

8:15 Paper 75b: A CFD Based High-Dimensional Deep Neural Network Surrogate Model for Oil/Water Separation in Horizontal Oil Production Pipelines

— Kuochen Tsai

8:30 Paper 75c: Polymer Drag Reduction in Taylor-Couette Flow: Routes for Improved Shear Stability

— **Stefanos Michaelides**, Thibaut Charpentier, Mark Wilson, Paul Hunt, Helen Sarginson, David Harbottle

8:45 Paper 75d: An Automated Microfluidic System for High Throughput Mechanistic Study of Asphaltenes Deposition and Dissolution in Porous Media Using *in Situ* Spectroscopy

- Weit Chen Topy Guo Yoogsh

— **Weiqi Chen**, Tony Guo, Yogesh Kapoor, Andrew Yen, Nikhil Joshi, Ryan L. Hartman

9:00 Paper 75e: Modeling Asphaltene Deposition in Production Pipelines

— Ahmed Al-hosani, Nagu Daraboina

9:15 Paper 75f: Effect of Asphaltenes
on the Structure and Surface Properties

of Wax Crystals in Waxy Oils

— *Huiyong Xue*, *Jinjun Zhang*

9:30 Paper **75g**: Paraffin Deposition Modeling – Is the Current Methodology Sufficient?

— **Yingda Lu**, Jinghao Yang, Cem Sarica, Elijah Bell, Nagu Daraboina **9:45 Paper 75h:** The Influence of Nanocomposite Pour Point Depressant on Wax Deposition of Waxy Oil

— Chuanshuo Wang, Wei Wang, Huirong Huang, Zeheng Peng, Jing Gong, Yanfen Ding

10:00 Paper **75i**: Phase Equilibrium Conditions of Methane Hydrate in Presence Aqueous Solutions of CaBr₂, MgBr, and ZnBr,

— **Dnyaneshwar Bhawangirkar**, Jitendra Sangwai

10:15 Paper **75j**: Evaluation of Pyrite Scale Reaction Kinetics in a Rotating Disk Apparatus Using Chelating Agents and a Converter

— Ibnelwaleed Hussein, **Musa Eltayeb Musa Ahmed**, Abdulmujeeb Onawole

(76) Fundamentals of Environmental Kinetics and Reaction Engineering

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Blue Spring I/II Hyun-Tae Hwang, Chair Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by: Fundamentals

8:00 Paper 76a: Kinetic Parameter Estimation from Experimental Laboratory Data for Modeling Reactions Occurring in a Groundwater Permeable Reactive Barrier

— Matthew Alexander, Avinash Kumar

8:25 Paper 76b: Pyrolytic Remediation of Petroleum-Contaminated Soil in a Pilot-Scale Rotary Kiln Reactor: Reaction Mechanisms, Soil Transformations and Treatment Intensity Tradeoffs

— Wen Song, Julia E. Vidonish, Pedro J. J. Alvarez, **Kyriacos Zygourakis**

8:50 Paper **76c:** Nitrate Reduction By Catalytic Hydrogenation: Controlling Hydrogen Delivery with Nano-Enabled Polymeric Hollow Fibers

— **Juliana Levi**, Sujin Guo, Shalinee Kavadiya, Yiyuan Yin, Ariel J. Atkinson, Zachary Holman, Bruce Rittmann, Michael S. Wong, Sergi Garcia-Segura, Paul Westerhoff

(77) Fundamentals of Fluidization Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 19 Mayank Kashyap, Chair Marc-Olivier Coppens, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

8:00 Paper: PTF SABIC Young Professional Award

8:30 Paper 77a: Fluidization of Graphene Nanoplatelets: From Microstructure to Hydrodynamics — *Damiano La Zara*, Fabio Grillo, J. Ruud van Ommen

8:50 Paper 77b: Bubble Self-Arrangement in Annular Gas-Solid Fluidized Beds

— Kaiqiao Wu, Victor Francia, Marc-Olivier Coppens

- **9:10** Paper 77c: Electrostatic Charging and Fluidization Behaviors of Dielectric Particles in the Presence of Noble Gases Guanhe Rim, Dongyi Wang, Sankaran Sundaresan, Ah-Hyung Alissa Park
- **9:30 Paper 77d:** An Immiscible Fluids Approach for Correctly Predicting Agglomerate Dynamics during Particle ALD
- Julia Hartig, Alan W. Weimer
- **9:50** Paper **77e**: Modeling Cohesive Gas-Particle Flows with a Parcel-Based Lagrangian Approach
- Stefan Radl, Josef Tausendschön
- **10:10 Paper 77f:** Rayleigh-Taylor Instability in Vibrated Gas-Fluidized Particles
- Christopher McLaren, Thomas M. Kovar, Alexander Penn, Christoph R. Müller, **Christopher M. Boyce**

(78) Fundamentals of Interfacial Phenomena I

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom J Gerold A. Willing, Chair Younjin Min, Co-Chair

Sponsored by: Interfacial Phenomena

- **8:00** Paper 78a: Surfactant-Polymer Association in Aqueous Solutions Samhitha Kancharla, Marina Tsianou, Paschalis Alexandridis
- **8:14 Paper 78b:** Extended Surfactants: Impact of Molecular Structure on Micellization
- **Andrew M. Bodratti**, Junce Cheng, Marina Tsianou, Paschalis Alexandridis
- **8:28 Paper 78c:** Thermodynamic Scaling Laws for Surfactant Interfacial Properties
- **Zachary R. Hinton**, Nicolas J. Alvarez
- **8:42** Paper 78d: Colloidal Depletion Forces in Solutions of Mutually Repelling Polyelectrolytes and Ionic Surfactants
- Bhagyashree Lele, Robert D. Tilton
- **8:56 Paper 78e:** Tensiometry, Interfacial Rheology, and Strain Field Mapping of Complex Interfaces
- **Mehdi Molaei**, Jiayi Deng, Nicholas G. Chisholm, John C. Crocker, Kathleen J. Stebe
- **9:10** Paper 78f: Rheology of oil-watersurfactant interfaces measured from mesoscopic simulations
- Micheline Abbas, Zhen Li
- **9:24** Paper **78g**: Rates of Replacement of Initially Oil-Filled Microscopic Cavities with Bulk Water
- Hans Larson, Jeong Woo Kim, **Donaiin Seo**
- 9:38 Paper 78h: Effect of Nature of Brine Solution on the Water-in-Crude Oil Interface for Low and High Tan Oil — Vikky Anand, Vinay Juvekar,
- **Vikky Anana**, Vinay Juvekai Rochish Thaokar
- **9:52** Break

10:06 Paper **78**j: Condensation Dynamics on Phase Switching Liquids — *Rukmava Chatterjee*, *Sushant Anand*

(79) Gene Regulation Engineering: Applications in Medicine and Biotechnology

Monday, Nov 11, 8:00 AM
Hyatt Regency Orlando, Celebration 14
Qing Sun, Chair
J. Andrew Jones, Co-Chair
Piyush Jain, Co-Chair

Albert Keung, Co-Chair Joseph Rollin, Co-Chair Kate E. Galloway, Co-Chair

Sponsored by: Bioengineering

- **8:00 Paper 79a:** Exploring Plant Phospholipase for Novel Antimicrobial Activities
- Shanhui Xu, Yanran Li, Curtis Chen
- **8:18** Paper 79b: Accelerating the Design and Engineering of Microbial Cell Factories Via Synthetic Biology and Automation
- **8:36 Paper 79c:** Programming Animal Physiology and Behaviors through Engineered Bacteria
- Baizhen Gao, Qing Sun

— Pu Xue

- **8:54** Paper 79d: Streamlined Assessment of Membrane Permeability: A Simple and Inexpensive High-Throughput Method for Multiple Applications
- **Miguel C. Santoscoy**, Laura R. Jarboe
- **9:12 Paper 79e:** Responsive Hydrogel Networks Controlled By Bacterial Metabolism
- **Austin J. Graham**, Adrianne M. Rosales, Benjamin K. Keitz
- **9:30 Paper 79f:** Conditional Protein Rescue (CPR) By Binding-Induced Protective Shielding
- Andrew Gaynor, Wilfred Chen
- **9:48 Paper 79g:** Invited Talk Gene Regulation Engineering
- Tamara L. Kinzer-Ursem

(80) Industrial Applications of Integrated Synthesis, Design and Operations Through Modeling and Optimization

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 17 Yihui Tom Xu, Chair Shaibal Roy, Co-Chair Prashant Kumar, Co-Chair

Sponsored by: Process Research and Innovation

- **8:00** Paper 80b: Model Based Plant-Wide Optimization of an Industrial Scale Continuous Tank Crystallizer Network for Dextrose Monohydrate Crystallization
- **Botond Szilagyi**, Kanjakha Pal, Iman Beheshti Tabar, Zoltan K. Nagy

- **8:21 Paper 80c:** Systematic Design and Intensification of Shale Gas Utilization Processes
- **Mohammed Sadaf Monjur**, Jianping Li, Salih E. Demirel, M. M. Faruque Hasan
- 8:42 Paper 80d: Evaluation of Helium Extraction Technologies While Considering Optimization and Integration with Nitrogen Rejection — Homa Hamedi, Iftekhar A. Karimi, Truls Gundersen
- **9:03 Paper 80e:** Kinetic Modeling and Process Control for the Preparation of Graphene Oxide
- **Chang Li**, Liming Shen, Ningzhong Bao
- **9:24** Paper 80f: High-Fidelity Modeling and Optimization of Natural Gas Dehydration and Liquid Recovery Plants *Dara Satyadileep, Yasser Al Wahedi,*
- Abdallah S. Berrouk, Simon Leyland
 9:45 Paper 80g: Bayesian
 Optimization Approach to Operation
 Recipe Optimization of Semi-Continuous
- **Dongwoo Lee**, Seongeon Park, Damdae Park, Jong Min Lee
- **10:06** Paper **80h:** Optimal Scheduling of Multi-Product Pipeline Distribution with Consideration of Comprehensive Transmix Handling for Petroleum Refineries

 Li Yu, Qiang Xu

(81) In Honor of Fabio H. Ribeiro's 60th Birthday (Invited Talks)

Monday, Nov 11, 8:00 AM
Hyatt Regency Orlando, Florida
Ballroom B
Viktor J. Cybulskis, Chair
James W. Harris, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00 Paper 81a:** Introductory Remarks By Session Chairs
- Viktor J. Cybulskis, James W. Harris
- **8:05** Paper 81b: First Principles Studies of Supported Heterogeneous Catalysts: Water-Gas Shift Reactivity at Metal/Oxide Interfaces
- Paulami Majumdar, Tej S. Choksi, Yanran Cui, Fabio H. Ribeiro, **Jeffrey Greeley**
- **8:30 Paper 81c:** A Resonant Inelastic X-Ray Scattering Study of Pt-Fe Intermetallic Compound Nanoparticles: Effect of Stoichiometry on the Valance Electronic Structure of Pt
- Evan C. Wegener, Brandon C. Bukowski, Zhenwei Wu, A. Jeremy Kropf, Guanghui Zhang, Jeffrey Greeley, **Jeffrey T. Miller**
- **8:55 Paper 81d:** Influence of Zeolite Framework on Cu Ion Mobility and the Kinetics of Selective Catalytic Reduction of Nitrogen Oxides with Ammonia
- **Rajamani Gounder**, William F. Schneider, Fabio H. Ribeiro, Jeffrey T. Miller, Casey Jones, Ishant Khurana, Sichi Li

- **9:20** Paper 81e: Structure, Dynamics, and Reactivity for Alkane Oxidation of Fe(II) Sites Situated in the Nodes of a Metal-Organic Framework
- Matthew C. Simons, Jenny G. Vitillo, Melike Babucci, Adam Hoffman, Michelle Beauvais, Zhihengyu Chen, Christopher Cramer, Karena W. Chapman, Simon R. Bare, Bruce Gates, Connie C. Lu, Laura Gagliardi, Aditya
- **9:45** Paper 81f: C-H Bond Activation and Light Alkane Dehydrogenation Catalysis: Oxidative and Non-Oxidative Routes and Equilibrium Shifting Via Tandem H₂ Oxidation Reactions

 Enrique Iglesia
- **10:25 Paper 81g:** Closing Remarks By Honoree
- Fabio H. Ribeiro

(82) Integrating Municipal, Food, and Industrial Waste into Biorefineries

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Regency Ballroom U Chenlin Li, Chair Hasan K. Atiyeh, Co-Chair Emmanuel Revellame, Co-Chair

Sponsored by: Sustainable Biorefineries

- **8:00 Paper 82a:** Bioconversion of Whey Lactose to Acetate and Propylene Glycol Deicers
- **Alexander P. Mathews**, Sathyanarayanan Sevilimedu Veeravalli
- **8:25** Paper 82b: Process Design, Techno-Economic Assessment and Environmental Impacts of Succinic Acid Production from the Organic Fraction of Municipal Solid Waste
- **Dimitrios Ladakis**, Eleni Stylianou, Sofia Maria Ioannidou, Chrysanthi Pateraki, Carol Sze Ki Lin, Apostolis Koutinas, Ioannis Kookos
- **8:50 Paper 82c:** Bioprocess Design and Techno-Economic Evaluation of 2,3-Butanediol Production from Crude Glycerol and Sugar-Based Feedstocks **Apostolis Koutinas**, Sofia Maina,
- Apostolis Koutinas, Sofia Maina, Eleni Stylianou, Olga Psaki, Aline Machado de Castro, Endrit Dheskali, Ioannis Kookos
- **9:15 Paper 82d:** Design and Analysis of the Integrated Process for Algae Conversion to Mix Alcohols
- Yue Zhang**, Abhay Athaley**, Marianthi lerapetritou
- **9:40** Paper **82e**: Production of Value Added Co-Products from the Hydrothermal Liquefaction of Unhydrolyzed Solids
- **Vinod S. Amar**, Bharat Maddipudi, Anuj Thakkar, Katelyn Shell, Dylan Rodene, Tylor Westover, Sandeep Kumar, Ram B. Gupta, Rajesh Shende
- **10:05** Paper **82f**: Hydroxyl Group Stabilization for Increased Yields of Low Molecular Weight Products in the Co-Pyrolysis of Cellulose and Thermoplastics
- Melisa Nallar, Hsi-Wu Wong

(83) Managing in the High Tech World

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 18 Okiemute Sankey, Chair Fernando Aguirre, Co-Chair

Sponsored by: Management Division

8:00 Paper 83a: A Chemical Engineer's Overview of Artificial Intelligence and Machine Learning

- Austin S. Lin

8:25 Paper 83b: How Virtual Advisors Create Practical Employee Efficiency Boosts in the Chemical Engineering Workplace

- Alec Walker

8:55 Paper 83c: Global Teams: Technology & People — *Frank van Lier*

(84) Materials Synthesis and Processing with Compressed or Supercritical Fluids

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom L Christopher L. Kitchens, Chair Steven R. Saunders, Co-Chair

Sponsored by: High Pressure

8:00 Paper 84a: Synthesis and Processing of Polymers with Supercritical Fluids

- Nikhil Prakash, Amit Rai

8:17 Paper 84b: Supercritical Continuous Synthesis of Heterogeneous Nitrides Nanophotocatalysts

— Prasaanth Ravi Anusuyadevi, Cyril Aymonier, **Samuel Marre**

8:34 Paper 84c: Conversion of Magnesium Oxychloride to Chlorartinite with CO₂ and Resulting Increased Water Resistance

— **Christopher L. Kitchens**, Roque Góchez, Jim Wambaugh

8:51 Paper 84d: Supercritical Phase Inversion Technique to Produce Composite Membranes Cellulose Acetate-Levan

— **Antonio Tabernero**, Lucia Baldino, Álvaro González-Garcinuño, Stefano Cardea, Eva M. Martín del Valle, Ernesto Reverchon

9:08 Paper 84e: Supercritical Solvothermal Flow Synthesis of Advanced Nanostructured Materials — Cyril Aymonier, Marie Claverie, Diez-Garcia Marta, Martin François

9:25 Paper 84f: Alcohol Clustering Mechanisms in Supercritical Carbon Dioxide Using Diffusion NMR and Network Analysis

— **Steven R. Saunders**, Trent R. Graham, Daniel J. Pope, Yasaman Ghadar, Aurora E. Clark

9:42 Paper 84g: Green Pathways for Supercritical and Biphasic Extraction of Medically Active Components from Plant Biomass

- Kyle Cogswell, Aydin K. Sunol

9:59 Paper 84h: Deflagration and Pressure Relief of High-Pressure Ethylene and Ethylene-Vinylacetate-Mixtures on a Laboratory Scale

— Ömer Delibalta, Markus Busch

(85) Metabolic Engineering for Food, Feed, and Bioproducts

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 1 Nuttha Thongchul, Chair Chi Cheng, Co-Chair

Sponsored by: Food

8:00 Paper **85a**: N-Butanol Production in *Clostridium Tyrobutyricum* Overexpressing a Heterologous Hydrogenase

— **Weiming Li**, Chi Cheng, Guangli Cao, Nanqi Ren, Shang-Tian Yang

8:18 Paper **85b:** Metabolic Engineering of Filamentous Fungi Using the CRISPR/Cas_a Systems

— Xiao-Jun Ji

8:36 Paper **85c:** Engineering Escherichia coli for Production of Biochemicals from Acetate — Hao Yang, Bing Huang, Ningyu Lai,

Zhimin Li, Qin Ye, **Hui Wu**

8:54 Paper 85d: Lycopene Production from Fatty Acids By Fed-Batch Fermentation of Metabolically Engineered *Escherichia coli*

— **Na Liu**, Ya-Hue Soong, Dongming Xie

9:12 Paper 85e: Upgrading Acid Whey to Animal Feed Via Metabolic Engineering of *Yarrowia Lipolytica*

— Constantinos Katsimpouras, Junichi Mano, Nian Liu, John Hammond, Devin Currie, Gregory Stephanopoulos

9:30 Paper 85f: Engineering Modular Photosynthetic Microbial Consortia for Sustainable Biochemical Production

— **David N. Carruthers**, Xiaoxia (Nina) Lin

9:48 Paper 85g: Keynote: Cell and Process Engineering of *Clostridium Acetobutylicum* for Biobutanol Production

— **Chuang Xue**, Guangqing Du

(86) Metabolic Engineering of Non-Model Organisms

Monday, Nov 11, 8:00 AM
Hyatt Regency Orlando, Celebration 4
Mark Blenner, Co-Chair
Cong T. Trinh, Co-Chair
Arul Varman, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 86a: Engineering Exceptional Solvent Tolerance in *Yarrowia Lipolytica* for Novel Biocatalysis

— Caleb Walker, Cong T. Trinh

8:18 Paper 86b: Metabolic Engineering of an Acid-Tolerant Strain *Pichia Kudriavzevii* for Itaconic Acid Production

— **Wan Sun**, Nuno Pereira Mira, Zengyi Shao **8:36 Paper 86c:** Assessing the Metabolic Capabilities of the Yeast Issatchenkia Orientalis SD₁₀₈ and Its Application to Biochemical Production

— **Patrick F. Suthers**, Zia Fatma, Yihui Shen, Siu Hung Joshua Chan, Hoang Dinh, Joshua D. Rabinowitz, Huimin Zhao, Costas D. Maranas

8:54 Paper 86d: Development of a Non-Leaky Inducible System for Tunable Gene Expression in *Actinobacillus Succinogenes* 130 Z and Application for Increased Succinic Acid Production

— Dianna Long, Cheryl Immethun,

9:12 Paper 86e: Development of a Genetic Toolset for *Acinetobacter Baylyi* (ADP.), a Host for Lignin-Based Metabolic Engineering

Mark Wilkins, Rajib Saha

— **Bradley W. Biggs**, Stacy Bedore, Erika Arvay, Ellen Neidle, Keith E.J. Tyo

9:30 Paper 86f: Metabolic Engineering of Non-Model Yeast Cutaneotrichosporon Oleaginosus for Valorization of Lignin and Lignin-Derived Aromatics

— Allison Yaguchi, Michael Spagnuolo, **Mark Blenner**

9:48 Paper 86g: Exploiting Nature's Anaerobes to Accelerate Biomass Breakdown and Sustainable Chemistry — *Michelle O'Malley*

(87) Mixing in Rheologically Complex Fluids

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 32 Li Xi, Chair Haifeng Shi, Co-Chair

Sponsored by: North American Mixing Forum

8:00 Paper 87a: Dispersion and Coalescence in Liquid/Liquid Systems Stabilized with Nanoparticles

— Lena Hohl, Susanne Röhl, Matthias Kraume

8:21 Paper 87b: Thixotropic
Suspensions in Static Mixer: Comparison of Different Structure-Based Models
— Mohammadali Masoudian, Ravindra Aglave, Thomas Eppinger

8:42 Paper 87c: Using Thrust As an Indirect Measure for Mixing Efficiency of Submerged Propeller Agitators in Non-Newtonian and Viscoelastic Media

— **Markus Kolano**, Manuel Brehmer, Matthias Kraume

9:03 Paper 87d: Macromixing Characteristics of Viscous and Shear-Thinning Fluids in Rotor-Stator Spinning Disc Reactors

— **Arnab Chaudhuri**, Wyatt Winkenwerder, John van der Schaaf

9:24 Paper 87e: Computational Fluid Dynamics Modeling of Mixing and Reaction of High-Viscosity Liquids in a Continuous Flow Reactor

— **Corey Clifford**, Kevin Glunt, Hari C. Mantripragada, Brandon Hlavaty, Nasser Al Azri, Cliff Kowall, Robert Enick, Götz Veser **9:45** Paper 87f: Non-Invasive Detection and Assessment of Coronary Stenosis Using Mean Age of Blood Flow — Javad Hashemi, Shahab Ghafghazi, Shesh Rai, R. Eric Berson

10:06 Paper 87g: Further Studies on Optimization of Agitation in Suspension Polymerizers

— **Richard K. Grenville**, Jason J. Giacomelli, Benjamin Boyer

(88) Multiphase & Liquid Phase Reaction Engineering

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom E Joris W. Thybaut, Chair Onkar Manjrekar, Co-Chair Vaibhay Kelkar, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper **88a:** Simulation and Validation of Biodiesel Production in Liquid-Liquid Film Reactors Integrated with PES Hollow Fibers Membranes

— **Mario Andrés Noriega**, Paulo César Narváez Rincón, Alberto Claudio Habert

8:20 Paper 88b: Kinetic Model of Enzymatic Hydrolysis in Liquid – Liquid System for Continuous Processes — Sherly Rusli, Janna Grabowski, Matthias Kraume

8:40 Paper 88c: FT-IR & Spectra Deconvolution: A Fruitful Combination for *in-Situ* Process Monitoring in Homogeneous Catalysis

— **Kai U. Kuennemann**, Jens M. Dreimann, Dieter Vogt

9:00 Paper 88d: Experimental Study of the Convective Heat Transfer in Single Phase with $\mathsf{5X}_{_{\mathsf{S}}}$ Rod Bundle in LWR and SMR

— **Saud Aldawood**, Hayder Alnaseri, Muhna Alshammari, Muthanna H. Al-Dahhan

9:20 Paper 88e: Study the Effect of Gas Flow Velocity on the Heat Transfer Coefficients in the Pebble Bed Reactor (PBR) — *Muhna Alshammari*, *Hayder Al-Naseri*, *Muthanna Al Dahhan*

9:40 Paper 88f: Experimental Characterization of Trickle Bed Reactor for Glycerol Oxidation

— **Jainesh H. Jhaveri**, Sanjay M. Mahajani, Akkihebbal K. Suresh

10:00 Paper 88g: Studying Tertiary Amine Alkylation Kinetics with Step-Flow in a Plug Flow Reactor Using in-Line H-NMR Spectroscopy

— **Roel Kleijwegt**, Wyatt Winkenwerder, John van der Schaaf

(89) Multiscale and Coarse-Grained Modeling of Polymers

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 15 Doug R. Tree, Chair Christopher R. Iacovella, Co-Chair

Sponsored by: Polymers

- **8:00 Paper 89a:** A Versatile Coarse-Grained Approach for Simulating Multi-Component Polymers: Field-Accelerated Monte Carlo Simulation
- **Dong Meng**, Jing Zong
- **8:30 Paper 89b:** Parameterization of Coarse-Grained Models for Block Copolymers: Approaches to Simulating Real Polymer Systems
- **Sahar Zenoozi**, Jakin B. Delony, Peter J. Ludovice, Clifford L. Henderson
- 8:45 Paper 89c: Application of the Energy Renormalization Method to a Coarse-Grained Polymer Model with a Dissipative Potential
- **Lilian C. Johnson**, Frederick R. Phelan Jr.
- **9:00 Paper 89d:** A Systematic Multiscale Coarse-Grained Model of Actin Filament Networks
- **Sriramvignesh Mani**, Harshwardhan H. Katkar, Gregory A. Voth
- **9:15** Paper 89e: Modeling Inter-Colloidal Interactions Induced By Adsorption of Mobile Telechelic Polymers Onto Particle Surfaces
- Wenlin Zhang, Ronald G. Larson
- **9:30** Paper 89f: Performance Mechanisms of Viscosity Modifiers Using Coarse-Grained Molecular Dynamics *Joshua D. Moore, Arturo Carranza, Nathaniel A. Cain, Joseph E. Remias*
- **9:45 Paper 89g:** The Effect of Nucleoid Associated Proteins on DNA Supercoiling
- Katelyn Dahlke, Charles E. Sing
- **10:00 Paper 89h:** Unraveling Structural Motifs of Heterogeneous Chromatin through Coarse-Grained Modeling
- **Joshua Moller**, Joshua Lequieu, Juan de Pablo
- **10:15 Paper 89i:** Applications of the Telegraph Model for Nanochannel Confined DNA
- **Aditya Bikram Bhandari**, Kevin D. Dorfman
- (90) Novel Approaches to CO₂ Utilization
- Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Discovery 43 Amishi Kumar, Chair Rameshwar D. Srivastava, Co-Chair
- **Sponsored by:** Advances in Fossil Energy R&D
- **8:00 Paper 90a:** Carbonate Ceramics for the Reduction of Global Carbon Footprint
- Richard E. Riman, Daniel Kopp
- **8:21** Paper 90b: CO₂ Mineralization Kinetics of Portlandite-Enriched Cementing Systems Exposed to Flue Gases
- Gabriel Falzone, Iman Mehdipour, Erika Callagon La Plante, **Gaurav Sant**

- **8:42** Paper 90c: Implementation of Ion Exchange Processes on Industrial Waste Streams for CO, Mineralization
- **Abdulaziz Alturki**, Steven Bustillos, Erika Callagon La Plante, Dante Simonetti, Gaurav Sant
- **9:03 Paper 90d:** Concentrating Solar Power Based Conversion of Carbon Dioxide to Fuels
- **Jeffrey G. Weissman**, Codruta Zoican-Loebick
- **9:24** Paper 90e: Synergy of Biological and Chemical Processes for High-Efficiency CO₂ Capture and Utilization
 Wei Lino
- **9:45 Paper 90f:** Microwave Active Conductive Metal Oxides for CO₂ Dry Reforming of Methane
- **Christopher Marin**, Douglas R. Kauffman
- **10:06 Paper 90g:** Nano-Engineered Catalyst for the Utilization of ${\rm CO_2}$ in Dry Reforming to Produce Syngas
- **Shiguang Li**, Baitang Jin, Zeyu Shang, Xinhua Liang
- (91) Overcoming Hurdles for Women in Innovation and Entrepreneurship
- Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom N

Whitney L. Stoppel, Chair Anita Shukla, Co-Chair Julie N. Renner, Co-Chair

Sponsored by: Women in Chemical Engineering Committee (WIC)

- (92) Process Intensification and Modular Manufacturing: Modeling and Simulation
- Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 28 Ignasi Palou-Rivera, Chair Paul Yelvington, Co-Chair
- **Sponsored by:** Process Intensification & Modular Chemical Processing
- **8:00** Paper 92a: Pharmaceutical Process Intensification Via Continuous Manufacturing and the Role of Modeling and Simulation
- **Nima Yazdanpanah**, Celia N. Cruz, Thomas O'Connor
- **8:25 Paper 92b:** Modular Process Intensification for Carbon Capture Using Data Driven Optimization
- **Sun Hye Kim**, Héctor Octavio Rubiera Landa, Timothy Mitchell, Matthew Realff, Fani Boukouvala
- **8:50 Paper 92c:** Process Simulation Study of Sour Gas Sweetening Technologies for Distributed Resources
- **Shuang Xu**, Yushi Deng, Selen Cremaschi, Mario Richard Eden, Kylie Webb, Harrison Wright, Paul S. Dimick
- **9:15 Paper 92d:** Process Intensification Framework for Reactive Separation Systems
- **Yuhe Tian**, losif S. Pappas, Baris Burnak, Justin Katz, Efstratios N. Pistikopoulos

- **9:40** Paper 92e: Process Innovation and Intensification Using Building Blocks *Jianping Li*, *Salih E. Demirel, M. M. Faruque Hasan*
- **10:05 Paper 92f:** Modeling Intensification of Biomass Fast Pyrolysis through Autothermal Operation
- **Benjamin Caudle**, Maximilian B. Gorensek, Chau-Chyun Chen
- (93) Rational Catalyst Design II: Tuning Performance with Intermetallics, Bimetallics, and Alloys
- Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom D Shu Hu, Chair Giannis Mpourmpakis, Co-Chair
- **Sponsored by:** Catalysis and Reaction Engineering Division
- **8:00 Paper 93a:** Fundamental Understanding of Surface Reactivity of Non-Noble Metal Intermetallic Compound Catalysts to Control C–H and C=C Bond Activation in Alkane Dehydrogenation
- **Yang He**, Yuanjun Song, Siris Laursen
- **8:18** Paper 93b: Integrating the Identification of Active-Site Ensembles within Descriptor-Based Screening Protocols for Bimetallic Catalysts
- **Verena Streibel**, Tej S. Choksi, Luke Roling, Jonathan Snider, An-Chih Yang, Hassan AlJama, Alessandro Gallo, Thomas F. Jaramillo, Matteo Cargnello, Frank Abild-Pedersen
- **8:36** Paper 93c: Impact of Intermetallic Ni-Ga Phase on the Selective Hydrogenation of Acetylene in Excess Ethylene
- **Anish Dasgupta**, Haoran He, Kayla Maghirang, Michael J. Janik, Randall Meyer, Robert M. Rioux
- **8:54** Paper 93d: Ceria Supported Bimetallic Overlayer Catalysts to Aid in the Dry Reforming of Methane

 Teneil Schumacher
- **9:12** Paper 93e: Ni-Au Single Atom Alloys for the Selective Oxidation of Methacrolein with Methanol to Methyl Methacrylate
- **Georgios Giannakakis**, Antonios Trimpalis, Maria Flytzani-Stephanopoulos
- **9:30 Paper 93f:** Defects Engineering for Solar Fuel Harvesting Photoelectrodes
- Mingzhao Liu
- **9:48** Paper 93g: Exploring Cluster-Size Effect in Catalysis: DFT Insights on Hocoh Decomposition on *H*-BN Supported Pd₆ Sub-Nanometer Clusters
- **Roberto Šchimmenti**, Manos Mavrikakis
- **10:06 Paper 93h:** Influencing the Surface Morphology of Highly Dilute Alloy Surfaces: An *Ab Initio* Monte Carlo Approach
- Konstantinos Papanikolaou, Matthew Darby, Michail Stamatakis

- (94) Regenerative Engineering: Substrate-Derived Control of Cellular Behavior
- Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 8 Yusuf Khan, Chair Erika Moore, Co-Chair
- **Sponsored by:** Regenerative Engineering Society
- **8:00 Paper 94a:** Place Holder CTL Introduction
- Cato T. Laurencin
- **8:15** Paper 94b: Quantum-on-Demand Biofabrication of 3D Tissue Test Systems *Karen Burg*
- **8:50 Paper 94c:** Robustness of Cellular Signaling with Respect to Dosage

 Hadel Al Asafen. Prasad Bandodkar.

Sophia Carrell-Noel, Gregory T. Reeves

- **9:10** Paper 94d: Synergistically Enhance Bone Cell Proliferation and Osteogenesis on 3D-Printed Scaffolds Using Two-Dimensional Black Phosphorus and Graphene Oxide Nanosheets
- Xifeng Liu, A. Lee Miller II, Sungjo Park, Matthew George, Brian Waletzki, Haocheng Xu, Andre Terzic, Lichun Lu
- **9:30 Paper 94e:** Biological Response Precision-Controlled By Spherical Pores *Buddy Ratner*
- **9:50** Paper 94f: Correlation between Fluid Shear Stress and Morphological Behaviour of Valvular Endothelial Cells *Nandini Deb, Carla M. R. Lacerda*
- **10:10** Paper 94g: Metabolite-Based Modulation of Dendritic Cells for Developing Effective Immunotherapy Sahil Inamdar, Joslyn Mangal, Abhinav P. Acharya
- (95) Solid-Liquid Interfaces
- Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom M
- Laura L. E. Mears, Chair Kai Kristiansen, Co-Chair
- Sponsored by: Interfacial Phenomena
- **8:00** Paper **95a:** NMR Relaxation, Powder Wettability and Hansen Solubility Parameter Applied to Particle Dispersibility
- David Fairhurst, Ravi Sharma, Terence Cosgrove, Keith Sanderson, **Stuart W. Prescott**
- **8:15** Paper 95b: Advancing and Receding Contact Angles of Powders Measured in a Closed Column
 Minglu Li, German Drazer, Gerardo
- Minglu Li, German Drazer, Gerardo Callegari 8:30 Paper 95c: Effect of Surfactant
- Kinetics on Spreading of Aqueous Trisiloxane Solutions
- Mark Simmons
- **8:45** Paper 95d: Simulating Contact Angle Hysteresis Using Pseudo-Line Tensions in a Continuum Fluid Dynamics Approach
- **Ping He**, Chun-Wei Yao

- **9:00 Paper 95e:** Bubble Nucleation after Drop Impact on Micro-Nano Textured Surfaces
- **Navid Saneie**, Varun Kulkarni, Sushant Anand
- **9:15 Paper 95f:** Redox-Triggered Orientational Responses of Liquid Crystals to Ozone Gas
- **Nanqi Bao**, Tibor Szilvási, Manos Mavrikakis, Nicholas L. Abbott
- **9:30 Paper 95g:** Artificial Mosquito "Compound Eye" Lens with Tunable Multifunctionality By Liquid-Based Assembly Process
- **Donglee Shin**, Denise Neibloom, Michael A. Bevan, Joelle Frechette
- 9:45 Paper 95h: Stability of Supported Lipid Bilayers in High Adhesive Regime — Pierluigi Bilotto, Maximilian Lengauer, Laura L. E. Mears, Ulrich Ramach, Markus Valtiner
- **10:00** Paper **95i**: Examining the Effects of Surfactants on the Structural and Mechanical Properties of a Thermoresponsive Polymer Brush

 Isaac J. Gresham Joshua D. Willow
- Isaac J. Gresham, Joshua D. Willott, Tim J. Murdoch, Ben A. Humphreys, Edwin C. Johnson, Grant B. Webber, Erica J. Wanless, Andrew Nelson, Stuart W. Prescott
- **10:15** Paper 95j: Optimizing Multiple Beam Interferometry in the Surface Forces Apparatus: Novel Optics, Reflection Mode Modelling, Metal Layer Thicknesses, and Anisotropic Layers
- Kai A Schwenzfeier, Andreas Erbe, Claudia Merola, Pierluigi Bilotto, Maximilian Lengauer, Hsiu-Wei Cheng, Laura L. E. Mears, Markus Valtiner

(96) Solids Handling and Processing in Particulate Systems

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 21 Madhusudhan Kodam, Chair Pallavi Pawar, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- **8:00 Paper 96a:** Predicting Loss-in-Weight Feeder Performance Based on a Reduced Set of Material Property Measurements
- **Tianyi Li**, Yi Tao, Fernando J. Muzzio, Benjamin Glasser
- **8:18 Paper 96b:** Flow Characterization of Compressed Woody Biomass
- Ehsan Akbari Fakhrabadi, **Matthew Liberatore**, Jonathan J. Stickel
- **8:36** Paper 96c: DEM Study on the Effect of Particle Size Distribution on Jamming in a 3D Conical Hopper Ya Zhao, Ray Cocco, Shiliang Yang,

Jia Wei Chew

8:54 Paper 96d: Real-Time
Measurement of Volumetric Fill in a
Storage Vessel and Discharge Rate By
Stereoscopic 3D Optical Scanning
— Mohammad Barzegar, Gabe P.
Redding, Clive E. Davies, Luke Fullard,
Miles C. E. Grafton

- **9:12** Paper 96e: Optimization of a Bag Filling Production Line for Starch By Down Scaling to Laboratory Scale

 Gabrie Meesters, Tom Knobbe
- **9:30 Paper 96f:** Flow-Aided Pneumatic Conveying of Cohesive Dairy Powder
- Akeem Olaleye, Gavin Walker, Harry E.A. Van den Akker
- **9:48** Paper 96g: Measurement of Solid Mass Flow Rate Under Different Flow Regimes in Pneumatic Conveying By Non-Intrusive Acoustic Emission Detection
- **Peng Zhang**, Yao Yang, Zhengliang Huang, Jingyuan Sun, Jingdai Wang, Yongrong Yang
- **10:06 Paper 96h:** Saponin Removal from Bitter Quinoa Ecotypes in Spouted BEDS (SB)
- Carlos Ramiro Escalera, Carmen Carla Quiroga Ledezma, Luis Arteaga Weill

(97) Steal this Coursel: Electives and Novel Course Offerings

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 22 Jonathan E. Wenzel, Chair Troy Vogel, Co-Chair

Sponsored by: Undergraduate Education

- **8:00** Paper 97a: Steal This Elective: Applied Food Science and Engineering *Margot A. S. Vigeant*
- **8:15 Paper 97b:** CRISPR in the Curriculum: A Genetic Engineering Elective for Chemical and Biomedical Engineers
- Elif E. Miskioglu
- **8:30 Paper 97c:** Process Prototype Design and Fabrication
- Jonathan E. Wenzel
- **8:45 Paper 97d:** Building Computational Skills for Mathematical Modeling in Science and Engineering through an Interdisciplinary Elective Course
- Ashlee N. Ford Versypt
- **9:00 Paper 97e:** Enhancing Global Understanding of Sustainable Energy Needs By Running a Faculty-Led International Program
- Courtney A. Pfluger
- **9:15 Paper 97f:** Scientific Computing for Chemical Engineers in Python
- Benjamin J. Davis
- **9:30 Paper 97g:** Hands-on Training on Intensified Membrane Processes for Wastewater Treatment
- **Itzel Marquez**, Eduardo Sáez, Kim Ogden, Andrea Achilli
- **9:45 Paper 97h:** Training All Chemical Engineers in Computing and Data Science
- Alexander W. Dowling

(98) Student Design Competition Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 25

Sponsored by: Student Chapters Committee Liaison

(99) Student Paper Competition Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 29/30 Douglas K. Ludlow. Chair

Douglas K. Ludlow, Chair Keith M. Forward, Co-Chair

Sponsored by: Student Chapters Committee Liaison

(100) Student Paper Competition in Sensor Technology I

Monday, Nov 11, 8:00 AM
Hyatt Regency Orlando, Celebration 10
Qingshan Wei, Chair
Ariel Furst, Co-Chair
Stephanie McCalla, Co-Chair

Sponsored by: Sensors

- **8:00** Paper 100a: Triplet-Triplet Annihilation Upconversion-Based Nanosensors for Fluorescent Detection of Potassium *Megan Jewell, Meredith Greer, Alexandra Dailey, Kevin J. Cash*
- **8:18 Paper 100b:** Glucose-Responsive Nanoparticles Based on Enzymatic Sensors for Self-Regulated Insulin Delivery
- **Lisa R. Volpatti**, Morgan Matranga, Abel B. Cortinas, Robert Langer, Daniel G. Anderson
- **8:36 Paper 100c:** In Vivo Biosensing Platform for Detection of Complex Human Milk Oligosaccharides
- **Fatima Enam**, Thomas J. Mansell
- **8:54** Paper 100d: Protein Detection with Peptoid-Functionalized Carbon Nanotube Optical Sensors
- **Linda Chio**, Jackson Travis Del Bonis-O'Donnell, Mark A. Kline, Jae Hong Kim, Ian McFarlane, Ronald N. Zuckermann, Markita Landry
- **9:12 Paper 100e:** Label-Free QCM Immunobiosensor for Real-Time Detection of GFP Antigen Using IOS-1 Peptoid:
- Solomon Isu, Jesse Roberts, Sergio I. Perez Bakovic, Shannon L. Servoss, Lauren F. Greenlee
- **9:30 Paper 100f:** High-Throughput Assaying of Individual Host-Pathogen Dynamics in Influenza A Virus Infection Using Drop-Based Microfluidics
- **Geoffrey Zath**, Emma Loveday, Humberto Sanchez, Connie B. Chang
- **9:48** Paper 1009: Minimally Invasive Extraction of Plant DNA Via a Polymeric Microneedle Patch for on-Site Detection of Plant Pathogens
- Rajesh Paul, Amanda Saville, Jeana Hansel, Yanqi Ye, Carmin Ball, Alyssa Williams, Xinyuan Chang, Guojun Chen, Zhen Gu, Jean Ristaino, Qingshan Wei

- **10:06 Paper 100h:** Nanostructured Polymer Interfaces for Improved Lectin-Based Capture and Detection of Bacteria
- **Mohammadali Masigol**, Scott T. Retterer, Ryan Hansen

(101) Synthesis and Application of Inorganic Materials: Part I

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 16 Xueyi Zhang, Chair Praveen K. Thallapally, Co-Chair

Sponsored by: Inorganic Materials

- **8:00** Paper 101a: Understanding Oligomerization Steps in Zeolite Growth Using Density Functional Theory *Emily Freeman*, *Jeffrey D. Rimer*, *Giannis Mpourmpakis*
- **8:18 Paper 101b:** Organic-Free Route for the Synthesis of Hierarchical Zeolite ZSM-11 Catalysts
- **Rishabh Jain**, Aseem Chawla, Noemi Linares, Javier García-Martínez, Jeffrey D. Rimer
- **8:36** Paper 101c: Additive-Free Synthesis of Hierarchical Zeolites By Utilizing Aluminosilicate Gel Memory Safiya Khalil, Maryam Khaleel
- **8:54 Paper 101d:** Cooperation and Competition between Organic and Inorganic Structure Directing Agents Influences the Aluminum Arrangement in CHA Zeolites
- John R. Di Iorio, **Claire T. Nimlos**, Sichi Li, Casey Jones, Eduard Kunkes, Subramanian Prasad, Ahmad Moini, William F. Schneider, Rajamani Gounder
- **9:12** Paper 101e: Unravelling the Nature of the Active Sites in Bimetallic MOFs and Their Role in C-C Activation for Room Temperature Propylene Hydrogenation
- Amani Ebrahim, Sanjaya Senanyake, Donna Chen, Anatoly I. Frenkel, Deependra Shakya, Otega Otega Ejegbavwo, Rajesh Thayalan, Sharfa Farzandh, Amy Brandt, Kostas Vogiatzis, Natalia B Shustova
- 9:30 Paper 101f: Nanorod Metal Organic Framework (MOF) As a Luminescent Probe for Selective Detection of Carcinogenic Hexavalent Chromium in Aqueous Medium — Enoch K Adotey, Mehdi Amouei Torkmahalleh, Mannix P Balanay
- **9:48** Paper 101g: Linker Doping Strategy for Hybrid Zeolitic-Imidazolate Frameworks and Their Ultrathin Membranes for Tunable Gas Separations — Febrian Hillman, Hae-Kwon Jeong
- **10:06 Paper 101h:** Amino Acid-Based Metal Organic Frameworks: Synthesis, Characterization, and Potential Biomedical Applications
- **Sahin Demirci**, Aydin K. Sunol, **Nurettin Sahiner**

(102) Synthetic Biology: Design Principles and Tool Development in Gene Regulation

Monday, Nov 11, 8:00 AM
Hyatt Regency Orlando, Celebration 3
Kevin V Solomon, Co-Chair
Peng Xu, Co-Chair
Leonidas Bleris, Co-Chair
Nicholas R. Sandoval, Co-Chair
Joseph Rollin, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 102a: An Ultrahigh Throughput Strategy for Extracellular Metabolite Screening By Combining *In Vivo* Biosensor with Microdroplet-Based FACS

- Yajie Wang, Vinh Tran, Huimin Zhao

8:18 Paper 102b: High-Throughput Approaches for Engineering Tunable Gene Expression Regulation in Non-Model Bacteria

— **Nicholas R. Sandoval**, Nancy Kim, Rochelle Joseph

8:36 Paper 102c: Engineering NAND and NOR Logic Gates Using Transcriptional Interference

— **Nolan O'Connor**, Antoni E. Bordoy, Anushree Chatterjee

8:54 Paper 102d: Harnessing Alternative Splicing for Gene Regulation in *Saccharomyces Cerevisiae*

— **Xiaoyi Cui**, Xiaoqiang Ma, Anthony J. Sinskey, Gregory Stephanopoulos, Kang Zhou

9:12 Paper 102e: Investigating Non-Coding Sequences with Regulatorlike Function on Pathway Expression Balance and Plasmid Stability Improvement

— **Carmen Lopez-Garcia**, Mingfeng Cao, Zengyi Shao

9:30 Paper **102f**: Analysis of Exponential Amplification Reaction (EXPAR) Termination and Overcoming with Looped Templates

— **Burcu Ozay**, Stephanie McCalla

9:48 Paper 102g: Engineered Autonomous Control of Metabolic Pathways

- Kristala Jones Prather

(103) Synthetic Fuels Production from Natural Gas and Hydrogen

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Regency Ballroom P

Maxim Lyubovsky, Chair

Sponsored by: Synthetic & Renewable Fuels

8:00 Paper 103a: Shell Gas-to-Liquids — *Joseph B. Powell, Leendert Bezemer*

8:30 Paper 103b: Challenges and Opportunities in Small-Scale Gas-to-Liquids (GTL) Processing

— Steve LeViness

9:00 Paper 103c: Green Technology Solutions for Synthetic Fuels — *Eli Philipp*, *Adam Paschal, Tobias Birwe* **9:30 Paper 103d:** Innovation for Direct Use of Ammonia in the Energy Market

— Shigeru Muraki

10:00 Paper **103e**: Methanol – a Practical Transportation Fuel for Today and Tomorrow

— Lawrence Navin, Gregory Dolan

(104) Topical Plenary: Microbial Interactions with Biomaterials and Host Cells (Invited Talks)

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Celebration 9 Angela C. Brown, Co-Chair Elizabeth J. Stewart, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

8:00 Paper 104a: Opening Remarks for Microbes at Biomedical Interfaces

— *Elizabeth J. Stewart*

8:05 Paper 104b: Invited Speaker: Innate Immunity at the Biomaterial Interface

— Brian A. Pettygrove, Rachel M. Kratofil, Jovanka M. Voyich, Kyler B. Pallister, Paul Kubes, **Philip S. Stewart**

8:33 Paper 104c: Invited Speaker: Structure, Stability, and Mechanics of Bacterial Communities Colocalized with Fibrin Network

— **Michael J. Solomon**, Tianhui (Maria) MA, J. Scott Van Epps

9:01 Paper 104d: Invited Speaker: Microbial Interactions with the Intestinal Mucosal Barrier: Impact of Lumen Stimuli

— **Rebecca L. Carrier**, Chia-Ming Wang, Jaclyn Lock, Taylor Carlson

9:29 Paper 104e: Invited Speaker: Controlling Bacterial Adhesion on Biomedical Interfaces with Bio-Inspired Liquid-Infused Surfaces

- Caitlin Howell

9:57 Paper 104f: Invited Speaker: Responsive Antibacterial and Antifungal Biomaterials for Infection Treatment

— Anita Shukla

(105) Undergraduate Research Presentations - Chemicals & Environment

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 31 Cory Thomas, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

(106) Unconscious Bias in Engineering: Why Is It Relevant to the Profession and What Can We Do

Monday, Nov 11, 8:00 AM Hyatt Regency Orlando, Bayhill 26 Cynthia Murphy-Ortega, Co-Chair Sindia Rivera-Jimenez, Co-Chair

Sponsored by: Engineering for Inclusion

(107) Networking Luncheon -Sponsored by WIC (Women in Chemical Engineering) (Ticketed Event)

Monday, Nov 11, 11:00 AM Hyatt Regency Orlando, Windermere

Sponsored by: Women in Chemical Engineering Committee (WIC)

11:00 Paper 107a: Luncheon Keynote Presentation

- Shelly R. Peyton

(108) Presidential Lecture Monday, Nov 11, 11:15 AM Hyatt Regency Orlando, Plaza International Ballroom H

Monty Alger, Chair
Sponsored by: Liaison Functions

11:15 Paper 108a: The Valence of Skills: The Rise of Hybrid Jobs

- Matt Sigelman

(109) Advances in Biosensors and Biodiagnostics: Biosensor and Biodiagnostic Detection Methods

Monday, Nov 11, 12:30 PM
Hyatt Regency Orlando, Celebration 4
Kevin J. Cash, Co-Chair
Xiao-an Fu, Co-Chair
Chang Liu, Co-Chair
Stephanie McCalla, Co-Chair
Hyun J. Kwon, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 109a: Transcriptional Biosensors That Discriminate between Radiation Sources

— **Molly Wintenberg**, Lisa Manglass, Nicole Martinez, Mark Blenner

12:48 Paper 109b: Competitive Protein-Based Fluorescent Biosensor for Glucose Detection in Exhaled Breath Condensate

— **Divya Tankasala**, Karin Ejendal, Tamara L. Kinzer-Ursem, Jacqueline Linnes

1:06 Paper **109c:** Engineering Thermostable Binding Protein rcSso₇d Against Zika Virus for Paper-Based Diagnostic Tests

— Ki-Joo Sung, Quinlan Johns, Hadley D. Sikes

1:24 Paper 109d: Block Optical DNA Sequencing and Content Scoring for Rapid Genetic Biomarker Identification — *Lee Korshoj, Prashant Nagpal*

1:42 Paper 109e: Rapid and Specific Genotyping for Blood Infection Identification

— William G. Pitt, Ryan L. Wood, Robert L. Hanson, Adam T. Woolley, Gopikrishnan G. Meena, Holger Schmidt, Aaron R. Hawkins

2:00 Paper 109f: Downconversion Luminescent Nanoparticles Harnessing Changes in the Surface Dipole As a Novel Approach for Small Molecule Detection

— **Khashayar R. Bajgiran**, James A. Dorman, Adam T. Melvin

2:18 Paper 109g: Nano Field-Effect Transistor-Based Biosensors for Healthcare

— Ashok Mulchandani

(110) Advances in Computational Methods and Numerical Analysis Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 26 Jinfeng Liu, Chair Sivaraman Ramaswamy, Co-Chair Dhruv Gupta, Co-Chair Kamil A. Khan, Co-Chair Matthew D. Stuber, Co-Chair Stevan Dubljevic, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

12:30 Paper **110a**: Sensitivity Analysis of Discontinuous Dynamical Systems — *Matthew R. Billingsley*, Paul I. Barton

12:46 Paper **110b**: Multilevel Monte Carlo Sampling for Thin Film Deposition Under Uncertainty

— **Grigoriy Kimaev**, Luis A. Ricardez-Sandoval

1:02 Paper 110c: Multiscale Three-Dimensional CFD Modeling and Reactor Design for ALD of SiO₂ Thin-Films — Yichi Zhang, Yangyao Ding, Yi Ming Ren, Panagiotis D. Christofides

1:18 Paper 110d: Advances in Bounding and Comparison Methods for Dynamic Process Models

— Kamil A. Khan, Yingkai Song

1:34 Paper 110e: Multiscale Modeling of Porosity and Cell Wall Thickness of Wood Chips in Pulp Digester — Hyun-Kyu Choi, Joseph Sang-Il Kwon

1:50 Paper 110f: Computing Robust Controlled Invariant Sets of Nonlinear Dynamical Systems

— **Benjamin Decardi-Nelson**, Jinfeng Liu

2:06 Paper 110g: Pseudo-Transient Flowsheet Optimization Using Inertial Manifolds

— Calvin Tsay, Michael Baldea

2:22 Paper 110h: Discrete Output Regulation of Kuramoto-Sivashinsky Equation

— Junyao Xie, Stevan Dubljevic

2:38 Paper 110i: Learning Partial
Differential Equations from Discrete
Space Time Data: Convolutional and
Recurrent Networks, and Their Relations
to Traditional Numerical Methods
— Tom S. Bertalan, Felix Dietrich,

Thomas Thiem, Rob Farber, **loannis G. Kevrekidis**, Anthony Roberts

(111) Advances in Low-Cost Renewable Hydrogen Production at Large Scale

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Regency Ballroom P Eric Miller, Chair

Sponsored by: Synthetic & Renewable Fuels

12:30 Paper 111a: RE-Fueling the Future: Hydrogen As Critical Intermediate in Renewable Energy Conversion into Fuels

— Maxim Lyubovsky

1:00 Paper 111b: Future Role of Hydrogen in Dense Energy Carriers and **Energy Storage**

- Joseph B. Powell

1:30 Paper 111c: H₂@Scale Evaluation of Market Opportunities for Water Splitting with Low Cost Clean Energy

— Richard Boardman

2:00 Paper 111d: Advancements in PEM Electrolyzers and Uses in the Renewable Energy Economy

– Monjid Hamdan

2:30 Paper 111e: Renewable Hydrogen & Methane Production - Integration, **Optimization and Cost Improvements**

- Kevin W. Harrison, Nancy Dowe

(112) Advances in Process Design I Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 25 **Emre Gençer, Chair** Qi Zhang, Co-Chair

Sponsored by: Systems and Process Design

12:30 Paper 112a: Synthesis of Efficient Retrofit Designs Using Procafd - **Anjan Tula**, Shuang Xu, Selen

Cremaschi, Mario Richard Eden, Rafiqul

12:49 Paper 112b: Stability Analysis of Bifurcations of Nonsmooth Differential-Algebraic Models for Dry Distillation Columns

- Suzane M. Cavalcanti, Paul I. **Barton**

1:08 Paper 112c: Efficient Polycrystalline Silicon Production - Cesar Ramírez, Edgar Martín-Hernández, Mariano Martín, Juan Gabriel Segovia-Hernández

1:27 Paper 112d: A 'valve-Free' Model for Dynamic Simulation of Pressure Swing Adsorption Processes That **Automatically Determines Near-Optimal Operational Policies**

- Taehun Kim, Michael Sees, Toni Kirkes, Chau-Chyun Chen, Joseph Scott

1:46 Paper 112e: An Exchanger-Centric Superstructure for Heat Exchanger **Network Synthesis**

— Sajitha K. Nair**, Iftekhar A. Karimi**

2:05 Paper 112f: An Exact Reformulation of the Superstructure **Optimization Problem**

— Smitha Gopinath. Amparo Galindo. George Jackson, Claire S. Adjiman

2:24 Paper 112g: Simultaneous Synthesis and Design of Reaction-Separation-Recycle Processes Using Rigorous Models

- Yingjie Ma, Zekun Yang, Nan Zhang, Jie Li

2:43 Paper 112h: The Fluxmax Approach: Integrated Process Synthesis and Heat Integration Exemplified for the Production of Hydrogen Cyanide

— Georg S. Liesche, Dominik Schack, Kai Sundmacher

(113) Area Plenary: Adsorption and Ion Exchange - In Honor of Celio Cavalcante (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Manatee Spring I

Stefano Brandani, Chair Peter I. Ravikovitch, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 113a: Adsorption of CO2 on High Silica Zeolites: Structural Defects and Differences between Adsorbent Samples

- Adam Vidoni, Peter I. Ravikovitch, Mobae Afeworki, David C. Calabro, Harry W. Deckman, Douglas Ruthven

12:48 Paper 113b: Using Adsorption Microcalorimetry and Manometry to Measure Useful Data for Adsorbent Screening and Process Design - Debora Maia, A. Eurico B. Torres,

Moises Bastos Neto, Célio L. Cavalcante Jr, Diana Azevedo

1:06 Paper 113c: Using Data Analytics to Find Promising Metal-Organic Frameworks for Adsorption Applications - Benjamin Bucior, Seulchan Lee, Yongchul G. Chung, Randall Q. Snurr

1:24 Paper 113d: The Role of Adsorption Processes in Lignin Biorefinery to Make Vanillin and Syringaldehyde

— Alirio Egidio Rodrigues, Elson

1:42 Paper 113e: Improved Process for Ultra-High Purity Nitrogen Production - Jeff Hufton, Garret Lau, Timothy C. Golden, Chris Suggit, Jon Levin

2:00 Paper 113f: Transport Coefficients in Commercial Beads Measured Using a Thermal Frequency Response Method - Roberto Mennitto, Male Holtermann,

Enzo Mangano, Stefano Brandani, Federico Brandani, Pluton Pullumbi

2:18 Paper 113g: MOFs for Sour Gas Treatment: Design Strategies and Stability Considerations

— Krista S. Walton

2:36 Paper 113h: HCI Removal from H₂ Gas By Adsorption on Hydrated Ion-Exchanged Zeolites

- Ravi Sharma, Julien Cousin-Saint-Remi, Gino Baron, Joeri Denayer

(114) Area Plenary: Leaders in **Biomaterials (Invited Talks)** Monday, Nov 11, 12:30 PM

Hyatt Regency Orlando, Celebration 5 Cole A. DeForest, Chair Kyle Lampe, Co-Chair Eun Ji Chung, Co-Chair

Sponsored by: Biomaterials

12:30 Paper 114a: Engineering Advanced Materials for Neural Regeneration

- Christine Schmidt

1:20 Paper 114b: Designing Dynamic Feedback into Cell-Material Interactions — Sarah C. Heilshorn

2:10 Paper 114c: Synthetic Hydrogels and Implications of Immune Responses in the Context of Tissue Engineering - Stephanie J. Bryant

(115) Area 8E Plenary: Electronic and **Photonic Materials: Industry and** Academia (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 15 James A. Dorman, Chair

Sponsored by: Electronics and

12:30 Paper 115a: Carbon-Based Photonics: An Industry Perspective – Carey Tanner

12:55 Paper 115b: Atomic Layer Processing of Ferroelectric, Phase Change, and Threshold Switching Materials for Next Generation Nonvolatile Memory Devices

1:20 Paper 115c: Applications of Atomic Layer Deposition in Nanoelectronic Systems

– Damon Farmer

- Karl Littau

1:45 Paper 115d: Chiral Nanocrystals and Metamaterials

- Vivian Ferry

2:10 Paper 115e: Neuromorphic Computing with the Redox Transistor A. Alec Talin

2:35 Paper 115f: Energy Transport Processes in Hybrid Perovskites - William A. Tisdale

(116) Biochemical Conversion **Processes in Forest/Plant Biomass Biorefineries**

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Discovery 47 Shijie Liu, Chair Xiao Zhang, Co-Chair

Sponsored by: Forest and Plant **Bioproducts Division**

12:30 Break

12:47 Paper 116b: Kinetic Modelling of Lignocellulose Hydrolysis at High Solids

- Antonio C. F. dos Santos. Jonathan C. Overton, Ryan Szeto, Kendra A. Erk, Nathan S. Mosier, Eduardo Ximenes. Michael R. Ladisch

1:04 Paper 116c: Fermentation of Xylose to Carboxylic Acids Under Low pH Conditions

— Alexander Mathews

1:21 Paper 116d: Comparison of Product Distribution, Content and Fermentability of Biomass in a Hybrid Thermochemical/Biological Processing

— **Laura Jarboe**, Zhanyou Chi, Xuefei Zhao, Tannon J. Daugaard, Dustin L. Dalluge, Marjorie R. Rover, Patrick A. Johnston, Andre Salazar, Miguel Chavez-Santoscoy, Ryan G. Smith, Robert C. Brown, Zhiyou Wen, Olga Zabotina

1:38 Paper 116e: Superior Performance Biodiesel from Biomass Hydrolysate Fusel Alcohols and Bio-Oils: Fatty Acid Fusel Esters (FAFE) and Combustion **Behavior**

- Somnath Shinde, Eric Monroe, Fang Liu, Arul M. Varman, Anthe George, Rvan Davis

1:55 Paper 116f: Fenton-Based Oxidation As a Pre-Treatment to Sugarcane Vinasse to Lower Inhibition to the Growth of Oleaginous Fungi - Cristiano Reis, Ana Karine Carvalho, Heitor Bento, Heizir De Castro

2:12 Paper 116g: Co-Culture of Filamentous Feed-Grade Fungi and Microalgae As an Alternative to Increase Feeding Value of Ethanol Coproducts - Cristiano Reis, Bo Hu, Aravindan Rajendran, Larissa D'Otaviano

2:29 Paper 116h: Anaerobic Co-Digestion of Swine Wastewater and Agricultural Residues for Biogas Production

- Sabarish Srinivasan, Jay Cheng, Qingfang Zhang

2:46 Paper 116i: Effect of Fenton Pretreatment on Cellulose Oxidation and Its Enzymatic Hydrolyzability — Jing Yang, Yu Zhang, Maobing Tu

(117) Carbon Nanomaterials Graduate Student Award Session

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Discovery 44 Anju Gupta, Chair Gozde Sultan Demirer, Co-Chair

Sponsored by: Carbon Nanomaterials

12:30 Paper 117a: Graduate Student Award: Investigating the Properties of Nanoparticles Containing Fullerene-like

- Kimberly Bowal, Jacob W Martin, Laura Pascazio, Markus Kraft

12:47 Paper 117b: The Impact of Carbonaceous Nanoparticles to Climate through Their Composition and Morphology

Georgios A. Kelesidis, Sotiris E. **Pratsinis**

1:04 Paper 117c: Award Session: Measuring the Accessible Surface Area within the Nanoparticle Corona Using Molecular Probe Adsorption

- Minkyung Park, Daniel P. Salem, Dorsa Parviz

- 1:21 Paper 117d: Multimodal Study of Biological Corona Structure and Dynamics on Single-Walled Carbon Nanotubes
- **Rebecca L. Pinals**, Darwin Yang, Alison Lui, Daniel J Rosenberg, Wendy Cao, Markita Landry
- **1:38** Paper **117e**: Process Safety Analysis for Ti₃C₂Tx Mxene Synthesis and Processing
- **Pritishma Lakhe**, Evan Prehn, Touseef Habib, Jodie L. Lutkenhaus, Miladin Radovic, M. Sam Mannan, Micah J. Green
- 1:55 Paper 117f: Measuring the Accessible Surface Area within the Nanoparticle Corona Using Molecular Probe Adsorption
- Minkyung Park, Daniel P. Salem, Dorsa Parviz, Xun Gong, Kevin S. Silmore, Tedrick Thomas Salim Lew, Duc T. Khong, Mervin C. Ang, Seonyeong Kwak, Mary B. Chan-Park, Michael Strano
- 2:12 Paper 117g: Role of Functional Ligands in Graphene Oxide/MoSe₂ Heterostructure(HS): Effects on Doping, Excitons and Transport
- **Tuhin Kumar Maji**, Samir Kumar Pal, Debjani Karmakar
- 2:29 Paper 117h: Repetitive Pool Boiling Runs: A Controlled Process to Form Reduced GO Surfaces from GO with Tunable Surface Chemistry and Morphology
- **Aniket Rishi**, Anju Gupta, Satish Kandlikar
- (118) CAST Director's Student Presentation Award Finalists (Invited Talks)
- Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 24 Benoit Chachuat, Chair Michael Baldea, Co-Chair
- **Sponsored by:** Computing Systems and Technology Division
- **12:30 Paper 118a:** Machine Learning-Based Predictive Control of Nonlinear Processes
- **Zhe Wu**, Anh Tran, Panagiotis D. Christofides
- **12:49 Paper 118b:** An Operator Theoretic Framework for Data-Driven Identification and Control of a Hydraulic Fracturing Process
- **Abhinav Narasingam**, Joseph Sang-II Kwon
- 1:08 Paper 118c: Performance Assessment and Modification of an Adaptive MPC for Closed-Loop Insulin Delivery Systems
- Iman Hajizadeh, Sediqeh Samadi, Mert Sevil, Mudassir Rashid, Nicole Hobbs, Rachel Brandt, Mohammad Reza Askari, Zacharie Maloney, Ali Cinar
- **1:27 Paper 118d:** Data-Driven Dissipativity-Based Control
- Wentao Tang, Prodromos Daoutidis

- **1:46** Paper **118e**: Pyosyn: A Collaborative Ecosystem for Process Design Advancement
- **Qi Chen**, Sunjeev Kale, Johnny Bates, Romeo Valentin, David E. Bernal, Michael Bynum, John D. Siirola, Ignacio E. Grossmann
- **2:05** Paper 118f: Building Block-Based Design and Intensification of Chemical Processes
- **Salih E. Demirel**, Jianping Li, M. M. Faruque Hasan
- 2:24 Paper 118g: Advanced Computational Methods for the Solution of Nonlinear Scheduling Problems with Time-Variable Electricity Prices
- Pascal Schäfer, Alexander Mitsos
- 2:43 Paper 118h: Design of Dynamic Experiments for Model Discrimination Under Uncertainty Using Gaussian Process Surrogate Models
- Simon Olofsson, Ruth Misener

(119) Catalysis with Microporous and Mesoporous Materials II: Liquid-Phase Reactions

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Florida Ballroom A

Nicholas Brunelli, Chair Unmesh Menon, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 119a:** Enhancing Acid-Base Cooperative Catalytic Activity of Aminosilica Materials through Tuning the Micropore Volume
- **Nicholas Brunelli**, Nitish Deshpande, Takeshi Kobayashi, Chi-Ta Yang, Eun Hyun Cho, Marek Pruski, Li-Chiang Lin
- **12:50 Paper 119b:** Catalysis in Tight Spaces: Confined Solvent Structures Influence Stability of Surface Intermediates during Alkene Epoxidation within Lewis Acid Zeolites
- **Daniel T. Bregante**, Jun Tan, Ami Patel, Zeynep Ayla, David Flaherty
- 1:10 Paper 119c: Synthetic Routes to Chemical Building Blocks from Formaldehyde over Lewis Acidic Molecular Sieves
- Viktor J. Cybulskis
- 1:30 Paper 119d: Effects of Intrapore Hydroxyl Density on Confined Water Structures and Ethanol Dehydration Kinetics within Microporous Brønsted Acids — Jason S. Bates, Brandon C. Bukowski, Jeffrey Greeley, Rajamani Gounder
- **1:50 Paper 119e:** Organic-Functionalized Molecular Sieves As Direct Acylation Catalysts
- Marcella Lusardi, Mark E. Davis
- **2:10 Paper 119f:** Intensifying Interaction of Glycerol Acetalization and Mass Transfer By Modified HY Zeolites
- Noppadon Sathitsuksanoh

- **2:30** Paper **119g:** Controlling Chemoselectivity in Aldol Reactions with Solid Catalysts
- Koushik Ponnuru, Armindo Carvalho, Friederike C. Jentoft

(120) Characterization of Engineered Particles and Nanostructured Particulate Systems

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 20 M. Silvina Tomassone, Chair Mohammad Azad, Co-Chair

Sponsored by: Particle Production and Characterization

- **12:30 Paper 120a:** Stoppers and Skins on Clay Nanotubes Help Stabilize Oilin-Water Emulsions and Modulate the Release of Encapsulated Surfactants
- **Olakunle Ojo**, Azeem Afarinmade, James Trout, Marzhana Omarova, Vijay T. John, Jibao He, Duy Nguyen, Arijit Bose, Donghui Zhang, Diane A. Blake, Yuri Lyoy
- **12:48** Paper **120b**: Large Area Monolayer Coatings for Janus Particle Production
- James F. Gilchrist, Jinghui Gao
- **1:06** Paper 120c: Magnetic Nanoparticle Characterization By Dark-Field Imaging and Bright-Field Absorbance
- **Abhinav Sannidhi**, Paul W. Todd, Thomas R. Hanley
- **1:24 Paper 120d:** Yolk-Shell Composite Nanostructured Electrodes for High Capacity Lithium-Ion Batteries
- M. Silvina Tomassone, Kurt Smith

(121) Charged and Ion-Containing Polymers II

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 11 Vivek Sharma, Chair Samanvaya Srivastava, Co-Chair

Sponsored by: Polymers

- 12:30 Paper 121a: Ion Transport in Block Copolymer Electrolytes: Understanding Ion Correlations from Molecular Dynamics Simulations
- Kuan-Hsuan Shen, Lisa M. Hall
- **12:42 Paper 121b:** The Role of Interfaces on Ion Conduction in Well-Aligned Thin Film Block Copolymer Electrolytes
- Peter Bennington, Daniel Sharon, Paul F. Nealey, **Shrayesh N. Patel**
- **12:54 Paper 121c:** Electrostatic Screening Effects in a Salt-Doped Polarizable Diblock Copolymer
- **Douglas Grzetic**, Kris Delaney, Glenn H. Fredrickson
- **1:06 Paper 121d:** Proton Conducting Sulfonated Poly(ionic liquid) Block Copolymers
- **Rui Sun**, Mahesh Agrawal, Yossef A. Elabd

- **1:18** Paper **121e:** Synthesis and Characterization of Polymers Containing Single-lon per Chain
- **Sangwoo Lee**, Sungmin Park, Chulsung Bae
- **1:30** Paper **121f:** Influence of Backbone Solvation on Polyelectrolyte Solution Transport Properties
- **Kyle M. Diederichsen**, Bryan D. McCloskey
- **1:42 Paper 121g:** The Effect of Host Miscibility and Polarity Contrast in Polymer Blend Electrolytes
- Bill Wheatle, Venkat Ganesan
- **1:54** Paper 121h: Gibbs Ensemble Monte Carlo Simulations of Oligo(ethylene oxide)/Salt Mixtures **Zhengyuan Shen**, *Qile Chen*, *Timothy P. Lodge*, *J. Ilja Siepmann*
- 2:06 Paper 121i: Effect of Inorganic Multivalent Nanocluster on the Complexation and Electric Charging of Neutral Polymer in Solution
- **Yingxi Elaine Zhu**, Manuela Ferreira, Benxin Jing
- **2:18** Paper 121j: Toward Convergence of Ionenes and High-Performance Polymers
- **Jason E. Bara**, Kathryn E. O'Harra, Irshad Kammakakam
- 2:30 Paper 121k: Balancing Processing and Performance in Commercial lonomers
- **Zachary R. Hinton**, Nicolas J. Alvarez
- 2:42 Paper 1211: Antibacterial Activity of Cationic Conjugated Oligo/ Polyelectrolytes Against Wild Type and Antibiotic-Resistant Bacteria
- **Ehsan Zamani**, Shudipto Konika Dishari

(122) Chemical Engineers in Medicine Plenary I (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 12/13

Leonard F. Pease III, Chair Swomitra Mohanty, Co-Chair

Sponsored by: Chemical Engineers in Medicine

- **12:30 Paper 122a:** Micro and Nanotechnologies for Precision Medicine
- Sumita Pennathur
- **1:15 Paper 122b:** A Membrane Biochip Platform for Molecular Biomarker Diagnostics
- Hsueh-Chia Chang
- **2:00** Paper 122c: Medical Applications of Microfluidics: From Blood Fractionation to Liquid Biopsy
 Ian Papautsky

(123) Complex Flows and Soft Mechanics (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom L

Jacinta C. Conrad, Chair Vivek Narsimhan, Co-Chair

Sponsored by: Fluid Mechanics

- **12:30** Paper **123a**: Collaboration and Competition between Active Sheets for Self-Propelled Particles
- Abhrajit Laskar, Oleg E. Shklyaev, Anna C. Balazs
- **12:55** Paper **123b**: Electroconvective Flows in Complex Fluid Electrolytes *Lynden A. Archer*
- **1:20 Paper 123c:** Why Is Everything Squishy?
- John C. Crocker
- **1:45 Paper 123d:** Braiding Nanoscale Fibers Using Capillary Forces
- Vinothan N. Manoharan
- **2:10** Paper 123e: Experimental and Theoretical Study of Bond Dissociation in Associative Polymer Flows
- **Bradley D. Olsen**, Michelle Sing, Irina Rasid, Niels Holten-Andersen
- 2:35 Paper 123f: Soft, Wet, and Sticky: Viscous Forces and Elasticity in Wet Adhesion
- Joelle Frechette

(124) Computational Solid State Pharmaceutics

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 7 Yuriy Abramov, Chair Dana Barrasso, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **12:30 Paper 124a:** Probing the Sensitivity of Point Charge Potentials in an Attempt to Improve Their Ability to Rank the Stability of Pharmaceutical Polymorphs
- Nathan Abraham, Michael R. Shirts
- **12:51 Paper 124b:** Crystal Structure Prediction Applications Going Beyond a Stable Form Selection
- **Yuriy Abramov**, Guangxu Sun, Yunfei Zhou, Mingjun Yang, Qiao Zeng, Zhe Shen
- 1:12 Paper 124c: Accurate and Efficient Lattice Energy Models for Industry-Oriented Crystal Structure Prediction — David H. Bowskill, Isaac J. Sugden, Constantinos C. Pantelides, Claire S. Adjiman
- 1:33 Paper 124d: How Many Ritonavir Cases Are Still out There? — Hanno Dietrich, Jacco van de Streek, Marcus Neumann
- 1:54 Paper 124e: A Comparison of Methods for Capturing Hydrate-Anhydrate Transition Thermodynamics Eric Dybeck, Andrew Thiel, Geoffrey Wood, Frank Pickard IV, Michael Schnieders

- **2:15 Paper 124h:** Genarris 2.0: A Random Structure Generator for Molecular Crystals
- Rithwik Tom, Imanuel Bier, Timothy Rose, Harriet O'Brien, **Noa Marom**
- **2:36** Paper **124**i: Crystal Structure Prediction in Lead Optimization Phase of Drug Discovery
- Anders Broo

(125) Continuous Crystallization Processes

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Coral Spring I/II Nima Yazdanpanah, Chair Christopher L. Burcham, Co-Chair

Sponsored by: Crystallization and Evaporation

- 12:30 Welcoming Remarks
- **12:33 Paper 125a:** Hollow Fiber Membrane-Based Continuous Crystallization Processes
- Dengyue Chen, Kamalesh K. Sirkar
- **12:54** Paper **125b**: Continuous Crystallisation Oscillatory Flow Platform for Protein Purification and Bio-Separation
- **Xiaoyu Li**, Huaiyu Yang, Wenqian Chen, Jerry Y. Y. Heng
- **1:15** Paper 125c: Implementation of Continuous Crystallization to Circumvent a Meta-Stable Liquid-Liquid Separation
- Christopher Wilbert, Carlos Pons-Siepermann, Dimitri Skliar, Benjamin M. Cohen, Patricia Cho, Eric M. Saurer, Jose E. Tabora
- **1:36 Paper 125d:** Comparison of Isolation-Free Continuous Crystallization Operations: Falling Film Solution Layer Crystallization and Confined Suspension Crystallization
- **Rafael Lopez-Rodriguez**, Matthew Harding, Kevin Girard, Steven Ferguson
- 1:57 Paper 125e: Integrated Continuous Crystallization and Spray Drying of Beclomethasone Dipropionate for Pulmonary Drug Delivery
- Gabriela D. Hadiwinoto, Philip C.L. Kwok, Henry H.Y. Tong, Si Nga Wong, Shing Fung Chow, **Richard Lakerveld**
- 2:18 Paper 125f: Continuous Crystallization Development for the Endto-End Manufacturing of Ciprofloxacin HCl in Refrigerator-Sized Modules
- **Gerard Capellades**, Clemence Neurohr, Helena Wiemeyer, Luke Rogers, Gregory Hammersmith, Kersten Rapp, David Brancazio, Allan S. Myerson
- 2:39 Paper 125g: Achieving Particle
 Size and Impurity Control for a
 Continuous Crystallization Process
 Using a Digital Design Approach
 Niall Mitchell, Christopher L.
 Burcham, Filipe Calado, Steven Myers

(126) Continuous Processing in Drug Substance

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 6 Jonathan McMullen, Chair Elcin Icten Gencer, Co-Chair Christopher H. Marton, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- 12:30 Paper 126a: Development of a Continuous Hydrogenation Process for Pharmaceuticals Using a Trickle Bed Reactor
- **Onkar Manjrekar**, Krishna Sharma, Brian Kotecki, Kaid Harper, Anuj A. Verma, Thaddeus Franczyk, Elie Chaaya, Moiz Diwan
- **12:51 Paper 126b:** Characterization of a Flow Hydrogenation System and Application to a Sensitive Reaction for Production of an Active Pharmaceutical Ingredient Intermediate
- Christopher Lippelt, Shawn Conway, David Del Valle, Jianxin Han, Matthew Kreilein, Christopher H. Marton
- 1:12 Paper 126c: The Application of Flow NMR Toward the Development of a Kinetic Model for Continuous Grignard Formation
- Charles D. Papageorgiou, Christopher Mitchell, Jacob Santos-Marques, Joseph R. Niemiroski, Michaela Marquez, Brian L. Marquez, David J. am Ende
- 1:33 Paper 126d: Application of a Dynamic Flow Reactor Platform for Data-Rich Experimentation of Complex Flow Reactions
- **Brian M. Wyvratt**, Jonathan P. McMullen
- **1:54 Paper 126e:** Scale-up of a Continuous Extraction Process for an Equilibrium-Limited Reaction
- **Eric G. Moschetta**, Michael T. Tudesco, Eric A. Voight
- **2:15** Paper 126f: A Virtual Plant for Synthetic Continuous Manufacturing Via Integrated Systems-Based Modeling
- Elçin İçten-Gençer, Andrew J. Maloney, XiaoXiang Zhu, Gerard Capellades, Matthew B. Beaver, Seth Huggins, Ayman Allian, Pablo Rolandi, Richard D. Braatz, Roger A. Hart, Shawn Walker
- **2:36 Paper 126g:** Starting the Road to Commercialization: Pharmacy on Demand (POD) Ciprofloxacin
- Luke Rogers, Dale Thomas, Esther Chen, Victor Schultz, Travis Hart, Carter Salz, Gerard Capellades, Clemence Neurohr, Helena Wiemeyer, Gregory Hammersmith, Kersten Rapp, David Brancazio, Allan S. Myerson, Timothy Jamison, Klavs F. Jensen

(127) CO₂ Use and Reuse Monday, Nov 11, 12:30 PM

Hyatt Regency Orlando, Challenger 41/42

Amishi Kumar, Chair Rameshwar D. Srivastava, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

- **12:30 Paper 127a:** Tale of an Ethane Oxidative Dehydrogenation Catalyst with Long and Stable Life Under Harsh Conditions
- Jadid E. Samad, Amit Goyal
- 12:51 Break
- 1:12 Paper 127c: Modular Electrocatalytic Processing for Simultaneous Carbon Utilization and Alkane Conversion
- Samgopiraj Velraj, Damilola A. Daramola**, Jason Trembly**
- **1:33 Paper 127d:** Process Intensification for Electrochemical Utilization of CO₂
- **Ayokunle Omosebi**, James Landon, Jesse G. Thompson, Kunlei Liu
- **1:54 Paper 127e:** Integrated Process of CO₂ Capture and Conversion to Alkyl Carbonates
- C. B. Panchal, Richard Doctor
- **2:15** Paper 127f: Electrochemical CO₂ Conversion to Valuable Chemicals Feng Jiao
- 2:36 Paper 127g: Highly Active, Robust 3D Interconnected Porous Oxide-Derived Copper Electrocatalysts for Selective Conversion of CO₂ into Fuels Thuy-Duong Nguyen-Phan, Douglas R. Kauffman
- (128) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains II

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Regency Ballroom V

Dharik Mallapragada, Chair Fengqi You, Co-Chair Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by: Sustainable Energy

- **12:30 Paper 128a:** Design of Sustainable Biofuel Supply Chains While Accounting for Spatial Variability of Nutrient Runoff and Ecosystem Services *Tapajyoti Ghosh*, *Bhavik R. Bakshi*
- **12:55 Paper 128b:** Three-Stage Design of Microalgae-Based Biofuel Supply Chain Using GIS
- **Seongwhan Kang**, Seongmin Heo, Matthew Realff, Jay H. Lee
- **1:20** Paper **128c**: GIS-Based Two-Stage Stochastic Facility Location Problem Considering Planting Plan Uncertainty *Neng Fan, Ou Sun*
- 1:45 Paper 128d: An Integrated Demand and Supply Modeling Approach for the Energy System Design of a New Urban Area
- **Zhihao Chen**, Styliani Avraamidou, Pei Liu, Zheng Li, Weidou Ni, Efstratios N. Pistikopoulos

- **2:10 Paper 128e:** Multi-Level Life Cycle Analysis Tool for Sustainable Energy Systems Modeling
- **Emre Gençer**, Sarah Torkamani, Francis O'Sullivan

(129) Developments in Electrochemical Reactors, Fuel Cells, and Electrolyzers

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Challenger 38/39

Jamie Holladay, Chair Oliver Gutierrez Tinoco, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

12:30 Welcoming Remarks

- **12:35** Paper **129a**: Understanding the Performance and Limitations of Membrane-Electrode-Assembly Architectures for the Electrochemical Reduction of CO.
- **Lien-Chun Weng**, Oyinkansola Romiluyi, Alexis T. Bell, Adam Weber
- 1:00 Paper 129b: Aqueous-Phase Hydrogenation of Aromatic Rings and Carbonyl Compounds in the Presence of Applied Potential
- Udishnu Sanyal, Laura C. Meyer, Jamie Holladay, Kelsey A. Stoerzinger, John L. Fulton, Donald M. Camaioni, Johannes A. Lercher, **Oliver Gutiérrez**
- 1:25 Paper 129c: Development of Pt-Based Electrocatalysts for the Upgrading of Biomass-Derived Compounds Via the Kolbe Reaction
- **Yang Qiu**, Juan A. Lopez-Ruiz, Evan Andrews, Jamie Holladay
- **1:50 Paper 129d:** Chemical Transformations Via Electrochemical Reduction of Organics to Products
- Jamie Holladay, Juan A. Lopez-Ruiz, Mal-Soon Lee, Udishnu Sanyal, Katherine Koh, Oliver Gutiérrez, Vassiliki-Alexandra Glezakou, Roger Rousseau
- 2:15 Paper 129e: Assessing the Feasibility of Conceptual Electrocatalytic Processes through Inverse Techno-Economic Modeling
- **Michael Orella**, Yuriy Román-Leshkov, Fikile Brushett
- **2:40** Paper **129f**: Electrochemical Oxidative Dehydrogenation (e-ODH) As a Process Intensification Platform in Shale Gas Upgrading
- Damilola A. Daramola, Samgopiraj Velraj**, Jason Trembly**
- 3:05 Concluding Remarks

(130) Digital Twin (Invited Talks) Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 28 Ignasi Palou-Rivera, Chair Nima Yazdanpanah, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Introductory Remarks

- **12:35 Paper 130a:** Digital Twin, Raising It out of the Realm of a Cliché
- **Amish Sabharwal**, Ian Willetts, Errol Jacob
- **1:05** Paper **130b**: Asset Optimization Software Suites to Drive Digitalization from Process Modeling to Optimization to Asset Optimization
- **Ajay Lakshmanan**, Benjamin Fischer
- **1:35 Paper 130c:** A General Digital Applications Platform
- **Costas C. Pantelides**, Frances Pereira, Penny Stanger, Yiming Yan
- **2:05** Paper 130d: Concept of Digital Twin and Digital Thread in the Chemical & Process Industry
- liro Esko, Ravindra Aglave
- **2:35 Paper 130e:** Digital Twin for Aluminum Smelting
- **Raghunathan Rengaswamy**, Venkataraman Narayanan Venkatesan, Danny Raj M, Abhishek Sivaram, Sanjay Vijayaraghavan, Ashok Gopinath

(131) Distillation Processes Fundamentals, Developments, and Applications

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Barrel Spring II Andrew W. Sloley, Chair

Sponsored by: Distillation and Absorption

- 12:30 Introductory Remarks
- 12:32 Paper 131a: A Methodology for Predicting the Performance of Batch Strippers in the Mass Transfer Limited Regime
- **Balamurali Sreedhar**, Patrick Au-Yeung, Sven Claessens, Greg Coco
- **12:55** Paper 131b: The Development of the Carbon Dioxide Removal and Water Recycling (COHO) System for Spacecarft *TRA-My Richardson*, *Darrell Jan*
- **1:20 Paper 131c:** Point Efficiency Data for Distillation Column Design at Elevated Liquid Viscosities
- **Raj Ganesh Manivannan**, Tony J. Cai, Ken C. McCarley, Anand N. Vennavelli, Sayeed Mohammad, Clint P. Aichele
- **1:45 Paper 131d:** Process Development for High Efficiency Cryogenic Air Separation Unit
- Hiroshi Tachibana
- 2:10 Paper 131e: Experimental and Numerical Study of the Mass Transfer Performances of Commercial Sulzer EX Structured Packing at High Driving Force Alberto Servia
- 2:35 Paper 131f: Separation Column Gamma Scans - Moving into a New Dimension
- Lowell Pless, Tony Cai
- 2:59 Concluding Remarks

(132) Division Plenary: Major Separations Challenges (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Manatee Spring II

Isaac Gamwo, Chair

Sponsored by: Separations Division

- **12:30 Paper 132a:** National Academies Report: A Research Agenda for Transforming Separation Science
 Joan F. Brennecke
- **1:15 Paper 132b:** Challenges and Advancements in Extraction Processes for the Recovery and Purification of Cannabidiol from Hemp
- **Greg DiCosola**, Bernardo Flores, Matt Zandi, Dan Parker
- **1:55 Paper 132c:** The Biorefinery Separations Challenge New Materials and Processes
- Sankar Nair

(133) Dynamics and Modeling of Particulate Systems: Discrete and Continuum

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 21 M. Silvina Tomassone, Chair Casey Q. LaMarche, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- **12:30** Paper **133a:** Effects of Rolling Friction, Cohesion and Size Distribution on the Shear Flow of a Binary Particle Mix
- **Jiecheng Yang**, Pongpumin Bunchatheeravate, Joseph W. Bullard, Jennifer S. Curtis
- 12:48 Paper 133b: Superquadric Particle Method for Non-Spherical DEM Simulation in Open Source Mfix: Development, Implementation and Verification
- **Xi Gao**, Jia Yu, Ricardo J.F. Portal, William A. Rogers
- **1:06** Paper 133c: Continuum Simulations of Dense Granular Flow and Model Assessment
- **Viraj Vilas Belekar**, Alberto Passalacqua, Theodore J. Heindel, Kushal Sinha, Shankar Subramaniam
- 1:24 Paper 133d: Coupled Computational Fluid Dynamics – Aerosol Dynamics Model for Prediction of Nanostructured Films in an Aerosol Chemical Vapor Deposition Reactor
- **Clayton Kacica**, Poom Sittisomwong, Anusha Kamath, Pratim Biswas
- **1:42 Paper 133e:** Predicting Pressure Filtration Performance By CFD-DEM Coupling Approach
- **Boyang Li**, Kerianne M. Dobosz, Haitao Zhang, Jessica D. Schiffman, Kostas Saranteas, Michael A. Henson
- **2:00** Paper 133f: On the Fast Fluidized Bed Simulations Using Recurrence CFD Firas Dabbagh, Stefan Pirker, **Simon Schneiderbauer**

- 2:18 Paper 133g: Sub-Grid
 Deconvolution Approach for Filtered
 Two-Fluid Models and the Application to
 Fluidized Beds
- Simon Schneiderbauer

2:36 Paper 133h: Slow Granular Flows in a Split-Bottom Couette Device

— Peter V. Dsouza. Prabhu R Nott

(134) Efficient Chemical Processing

of Lignin to Bioproducts and Biofuels Monday, Nov 11, 12:30 PM

Hyatt Regency Orlando, Regency Ballroom Q Bin Yang, Chair Arthur J. Ragauskas, Co-Chair Ning Sun, Co-Chair

Joshua Yuan, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

- **12:30** Paper **134a:** Elucidating Lignin Structure and Relationships from Naturally Variant Populus Trichocarpa *Nathan Bryant, Jin Zhang, Wellington Muchero, Yunqiao Pu, Arthur J. Raqauskas*
- **12:51 Paper 134b:** Separation of Lignin Streams after Alkali and Ionic Liquid Pretreatment Using Tangential Flow Filtration
- **Jipeng Yan**, Ling Liang, Isaac Fittssprague, Kenton Chung, Qian He, Todd Pray, Ning Sun
- 1:12 Paper 134c: Replacing Coal Used in Steelmaking with Biocarbon from Hydrolysis Lignin -Techno-Economic Evaluation
- **Juha Hakala**, Petteri Kangas, Martin Björnström, Timo Fabritius, Pertti Koukkari
- **1:33 Paper 134d:** Conversion of Sugarcane Bagasse to Bioenergy over a Metal Oxide Catalyst
- **Naijia Hao**, Arthur J. Ragauskas
- **1:54** Break
- 2:15 Paper 134f: Fast Catalyst Evaluation Using Pyro-GC-MS for Lignin Conversion to Chemicals and Fuels — Maoqi Feng, Bin Yang, Sandeep Kumar
- 2:36 Paper 134g: Molten Alkali Carbonates Pyrolysis of Lignin in Digestate for Phenolic Production — Yi Wei, Jianbing Ji, Fengwen Yu

(135) Emerging Antimicrobial Methods

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 9 Cesar de la Fuente-Nunez, Chair Huan Gu, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

12:30 Paper 135a: Leveraging UV-C LEDs Vs. Mercury-Based Lamps for Electronic Disinfection in Healthcare
— Norman Horn, Christian Davis

- **12:46** Paper **135b:** Invited Speaker: Thermal Mitigation of Biofilms *Eric Nuxoll*
- **1:02 Paper 135c:** Invited Speaker: Anti-Toxin Strategies As an Antibiotic Alternative
- Evan Koufos, Eric Krueger, En Hyung Chana, **Angela C. Brown**
- **1:18** Paper 135d: Invited Speaker: Peptide-Based Approaches to Treating and Preventing Fungal Infections *Amy J. Karlsson*
- **1:34** Paper 135e: Invited Speaker: Toward Computer-Made Antibiotics Cesar de la Fuente-Nunez
- 1:50 Paper 135f: Acid-Transforming Chitosan (ATC)/DNA Polyplexes to Eliminate Intracellular *Salmonella Typhimurium* infection
- **Julius Edson**, Weiping Chu, Steffen Porwollik, Michael McClelland, Young lik Kwon
- 2:06 Paper 135g: Invited Speaker: Eradicating Antibiotic-Tolerant Bacteria and Biofilms By Antimicrobial Modular Proteins Produced By Cell-Free Protein Synthesis
- Seok Hoon Hong
- 2:22 Paper 135h: Mechanical Vibrations at Resonance Frequency on Hydrophilic Substrates Enhances Biofilm Removal
- William Ballance, Inkyu Oh, Yang Lai, Mohamed Elhebeary, Taher Saif, Yuhang Hu, Hyunjoon Kong
- 2:38 Paper 135i: Block Copolymer Nanoparticles Remove Biofilms of Drug-Resistant Gram-Positive Bacteria By Nanoscale Bacterial Debridement
- Mary B. Chan-Park, Jianghua Li

(136) Emerging Applications in Electrochemical Separations (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom I Xiao Su, Chair Christopher G. Arges, Co-Chair

Sponsored by: Electrochemical Fundamentals

12:30 Paper **136a**: Shock Electrodialysis for Ion-Selective Water Purification

— Kameron Conforti, Mohammad A. Alkhadra, Tao Gao, Huanhuan Tian, **Martin Z. Bazant**

1:00 Paper 136b: Thermodynamics and Chemo-Mechanics of Electrosorption Electrodes for Separation Applications
— Stella Vujic, Yousuf Bootwala,
Wan-Yu Tsai, Nina Balke, Marta Hatzell,
Kelsey Hatzell

1:30 Paper 136c: The Impacts of Fixed Chemical Charge Location and Abundance on the Performance and Cost of Capacitive Deionization Systems

— **Roland Cusick**, Kyle Smith, Steven Hand, Xia Shang, Martina del Cerro, Akash Bhat, Jeremy Guest

- **2:00 Paper 136d:** Practical Applications of Electrokinetic Separations
- **Yupo J. Lin**, Lauren Valentino, Shu-Yuan Pan
- 2:30 Paper 136e: Electrochemically Modulated Mitigation of Acid Gas Emissions
- T. Alan Hatton

(137) Engineering in Cancer Biology and Therapy III: Drug Development and Delivery

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 1 Ebong Eno, Chair Shreyas Rao, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 137a: Diffusion-Based Delivery of Alpha-Particle Radiotherapeutics Effectively Controls Recurrent, Chemoresistant Triple Negative Breast Cancer

— **Stavroula Sofou**, Aprameya Prasad

12:48 Paper 137b: Novel Cytostatic Annexin A_s -Drug Conjugates for Cancer Treatment

— **Benjamin Southard**, Patrick McKernan, Alexis Woodward, Roger G. Harrison

1:06 Paper 137c: Synergistic and Multimodal Cancer Gene Therapy Using Viral/Nonviral Chimeric Vectors

— **Margaret Lugin**, Angela Fleischman, Young Jik Kwon

1:24 Paper 137d: Silica Gel Encapsulation of Ovarian Cancer Cells for Selection of Cells Exhibiting Both a Higher Propensity to Enter Quiescence and Enhanced Chemoresistance

— **Tiffany Lam**, Hak Rae Lee, Alptekin Aksan, Samira M. Azarin

1:42 Paper 137e: High Diffusive Peptides for Drug Carriers in Tumor Extracellular Matrix

— **Rashmi Mohanty**, Xinquan Liu, Jae You Kim, Xiujuan Peng, Sahil Bhandari, Jasmim Leal, Dhivya Arasappan, Dennis Wylie, Debadyuti Ghosh

2:00 Paper 137f: Longitudinal Tracking of Single Cells Reveals Drug Resistant Phenotypes in Cancer

— **Adity Pore**, Shamim Ahmmed, Swastika S. Bithi, Siva A. Vanapalli

2:18 Paper 137g: Invited: Engineering Targeted Drug Delivery Vehicles

— Debra Auguste

(138) Engineering in Development and Aging

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 3 David Umulis, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 138a: Engineering Approaches to Understanding the Role of Tau in Neurodegeneration

— Daniel Oseid, Evan Wells, Anne Robinson **12:48 Paper 138b:** Reprogramming of Liver Cells By Understanding and Re-Engineering Developmental Master Regulatory Gene Circuits (DRGC)

— **Tala Mon**, Iyan Warren, Saber Meamardoost, Natesh Parashurama

1:06 Paper 138c: Mechanical Wrapping By Smooth Muscle Directs Epithelial Morphogenesis in the Lungs — *Michael A. Palmer, Celeste M.*

1:24 Paper 138d: Interactions between β -Amyloid and α -Synuclein for Amyloid Co-Assembly

— Jason Candreva, **Edward Chau**, Margaret Rice, Jin Ryoun Kim

1:42 Paper 138e: Human
Cerebral Organoids As Models for
Neurodevelopmental Disorders and
Test-Beds for Therapeutic Strategies
— Dilara Sen, Alexis Voulgaropoulos,
G. Aneeshkumar Arimbasseri, Zuzana
Drobna, Albert Keung

2:00 Paper 138f: Automated Tracking of Age-Induced Neuromuscular Health Decline in *C. Elegans*

— Taslim Anupom, Mizanur Rahman, Siddhartha Gupta, Purushottam Soni, Hunter Edwards, Monica Driscoll, Nathaniel Szewczyk, **Siva A. Vanapalli**

2:18 Paper 138g: Modulation of Transcriptional Kinetics Via Protein-DNA Interactions

— **Bomyi Lim**, Samuel Keller, Siddhartha Jena

(139) Environmental Division Awards and Honors (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Blue Spring I/II Debalina Sengupta, Chair Sally Ng, Co-Chair

Sponsored by: Environmental Division

12:30 Paper **139a:** Time for a Paradigm Shift: Toward an Engineering that Accounts for People and the Planet — *Bhavik R. Bakshi*

1:30 Paper 139b: Community-Engaged Environmental Measurements

— Kerry Kelly

(140) Experimental Investigation of Fluidization Processes

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 19 Greeshma Gadikota, Chair Sarah E. Mena, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

12:30 Paper 140a: Study of Hydrodynamic Behavior in a Shallow Rectangular Spouted Bed with Ascending Gas Flow Using Bed Pressure Signals and Image Analysis

— Jingsi Yang, **Ron Breault**, Justin Weber, Steven Rowan

12:55 Paper 140b: Effect of Baffles on the Flow Regime, Transition Velocities and Void Characteristics in a 6 in. Diameter Fluidized Bed

- Shyam Sundaram

1:20 Paper 140c: Hydrodynamic Analysis of Spouting Characteristics in a Slot-Rectangular Spouted Bed Reactor — Steven Rowan, Ronald W. Breault, Narasimhan Soundarrajan, Jingsi Yang, Samuel Bayham

1:45 Paper 140d: Development,
Validation and Application of a New
Methodology for the Measurements of
Particle Stresses in an Aerated Bed
— Lyes Ait Ali Yahia, Tobias Piepke,
Ross Barrett, Raffaella Ocone

2:10 Paper **140e**: What Can the FT₄ Do for Fluidized Solids Characterization?

— *Ben Freireich*, *Tim Freeman*, *Jamie Clayton*

2:35 Paper 140g: Advancing Cross-Scale Characterization of Reactive Fluid-Solid Interactions: Accelerated Carbon Mineralization for Integrated CO₂ Capture, Utilization and Storage — Greeshma Gadikota, Meishen Liu

(141) Exploring Ethical Dilemmas in the Workplace: Workshop

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 18 Joseph J. Cramer, Chair Okiemute Sankey, Co-Chair

Sponsored by: Professional Development

12:30 Paper 141a: Ethical Dilemmas - an Introduction

— Deborah Grubbe

1:00 Paper 141b: Data: Yours? Mine? Ours? and When Is Enough Enough? — *Gayle Gibson*

1:20 Paper 141c: Challenges Unique to the Biomedical & Biochemical Industry

Joseph Cramer

1:50 Paper 141d: Workshop: Dealing with Ethical Dilemmas

— Joseph Cramer, Okiemute Sankey

2:30 Paper 141e: Post-Workshop: Discussion

— **Joseph Cramer**, Okiemute Sankey

(142) Free Forum on Engineering Education: Junior and Senior Years I Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 23 Jennifer Pascal, Chair Aravind Suresh. Co-Chair

Sponsored by: Undergraduate Education

12:30 Paper **142a**: A Co-Teaching Approach to Unit Operations and Capstone Design - Joint Projects — *Jennifer Pascal*, *Daniel D. Burkey*

12:48 Paper **142b**: Undergraduate Chemical Engineering Laboratory: A Senior Capstone Experience

— David M. Griffin, Mark B. Shiflett

1:06 Paper 142c: Wastewater to Beer: An IPA for the EPA

— **Vance Jaeger**, Jim Watters, Milad Ebrahimi

- **1:24** Paper 142d: Chemical Engineering Lab for Seniors at United States Military Academy
- Matthew Armstrong, **Corey James**, Andrew Biaglow, Enoch Nagelli, Andrew Pfluger
- 1:42 Paper 142e: Applying PBL Methodologies to the Chemical Engineering Courses: Unit Operations and Modeling and Simulation, Using a Joint Course Project
- Miguel A. Ballesteros, Miguel A. Daza, Juan P. Valdés, Nicolas Ratkovich, Luis H. Reyes
- **2:00** Paper 142f: Developing Chemical Engineering and Analytical Science Acumen through Optimization of the Chocolate Process
- **April Miller**, Matthew Armstrong, Enoch A. Nagelli
- 2:18 Paper 142g: Using
 Multidimensional Metrics to Assess
 Changes to Student Attitudes and Ability
 in a Capstone Laboratory Sequence
 Gregory T. Neumann, Daniel
 Anastasio, Heather C. S. Chenette

(143) Fundamentals of Catalysis I Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom D

International Ballroom D
Thomas J. Schwartz, Chair
Casey O'Brien, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 143a:** Coverage-Dependent Adsorption of Hydrogen on Fe(100): Using Lattice Gas Parameters As Design Variables to Enhance Fe's Resistance to Oxidative Deactivation
- **Alyssa Hensley**, Greg Collinge, Jacob Bray, Jean-Sabin McEwen
- 12:48 Paper 143b: The Fate of Oxygen during Light Alkane Reforming, Oxidative Dehydrogenation, and Combustion
- Petar Lachkov, Rui Yao, **Ya-Huei** (Cathy) Chin
- 1:06 Paper 143c: The Proximity Effects and the Role of Molecular Shuttles in Water-Gas Shift and Methanol Synthesis
- **Stephanie Kwon**, Ting Chun Lin, Enrique Iglesia
- **1:24** Paper **143d**: Mechanistic Details of Vinyl Acetate Synthesis Reaction on Monometallic Pd Catalysts and the Influence of Cu Co-Catalysts
- Zhaoru Zha**, Prashant Deshlahra**
- **1:42** Paper 143e: Effects of Component Segregation in Bimetallic Alloy Catalysis *Konstantinos Goulas*
- **2:00 Paper 143f:** Study the Hydration Behavior of Surface Metal Oxide Species Via in-Situ Vibrational Spectroscopy
- **Hedun Wang**, Thu Nguyen, George Tsilomelekis

- 2:18 Paper 143g: The Effect of Promoters on Catalytic Activity of Supported V₂O₅-WO₃/TiO₂ Catalysts for Selective Catalytic Reduction (SCR) of NO with NH₃
- Mingyu Guo, Jun-Kun Lai, Michael Ford, **Israel E. Wachs**
- **2:36** Paper 143h: Selectivity in Multiple Guises: DFT and Microkinetic Models of NH₃ Catalytic Oxidation
- **Hanyu Ma**, William F. Schneider

(144) Fundamentals of Interfacial Phenomena II

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom J Gerold A. Willing, Chair Younjin Min, Co-Chair

Sponsored by: Interfacial Phenomena

- **12:30 Paper 144a:** Impact of Surface Roughness on Estimating Hamaker Constants through Non-Contact Atomic Force Microscopy
- **Michael C. Stevenson**, Stephen P. Beaudoin, David S. Corti
- **12:44** Paper **144b**: Effects of Interfacial Polymer Co-Adsorption on the Spontaneous Emulsification in the Presence of Asphaltenes
- **Mariana Rodriguez-Hakim**, Simone Bochner de Araujo, Zhen Yao, Gerald G. Fuller
- **12:58 Paper 144c:** Steric Hindrance Effect on Adsorption Kinetic of Asphaltenes on Oil/Water Interfaces
- **Shaghayegh Darjani**, Vincent Pauchard, Joel Koplik, Sanjoy Banerjee
- 1:12 Paper 144d: Phase Behavior, Micelle Structure and Stepwise Drainage of Aqueous Sodium Naphthenate Foam Films
- Shang Gao, Chrystian Ochoa, Vivek Sharma, **Samanvaya Srivastava**
- **1:26 Paper 144e:** Surfactant Migration on Polymeric Substrates
- **Jona Ramadani**, Daryl Williams, Mariangela Caputi, Ilaria Ambrogio
- **1:40 Paper 144f:** Bubble Spreading on Porous, Aerophilic Polymer Films
- **Aadithya Kannan**, Ping Gao, Jan Zawala, Gerald G. Fuller
- **1:54** Paper 144g: Quantitative Scaling Analyses for Estimating Domain Sizes and Compositions at Particle Surfaces By Surface-Enhanced NMR
- **Nathan A. Prisco**, Arthur C. Pinon, Brennan J. Walder, Lyndon Emsley, Bradley F. Chmelka
- **2:08 Paper 144h:** Design of Encapsulated Systems for Controlled Release
- **Luqing Qi**, Carol Mohler, Daniel Dermody, Arash Nowbahar, Casie Hilliard, Ray Drumright, Erin Vogel
- 2:22 Paper 144i: Molecular Adsorbate-Triggered Orientational Transitions of Liquid Crystals on Metal Surfaces
- **Tibor Szilvási**, Jake Gold, Huaizhe Yu, Nanqi Bao, Nicholas L. Abbott, Manos Mavrikakis

- 2:36 Paper 144j: Accelerated Molecular Dynamics Investigation of the Rapid Diffusion of Large Heteroepitaxial Islands
- **Obioma U. Uche**, Danny Perez, Arthur F. Voter, John C. Hamilton

(145) Industrial Internet of Things (IIoT) in Process Manufacturing and Beyond

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 27 Zhenyu Wang, Chair Tim Olsen, Co-Chair

Sponsored by: Next-Gen Manufacturing

- **12:30** Paper **145a:** Transforming Abundant Data into Improved Process Reliability (Keynote Talk)
- Tim Olsen
- **1:00 Paper 145b:** Going Digital in Downstream (Keynote Talk) *Cindy Crow*
- **1:30** Paper **145c:** Emission Monitoring and Plant Integrity Enhancement

 Helen Lou, *Huilong Gai*
- **1:50** Paper **145d**: Optimizing Real-Time Spatiotemporal Sensor Placement for Monitoring Air Pollutant for Health Impact Assessment
- **Rajib Mukherjee**, Urmila M. Diwekar, Coco Liu
- **2:10 Paper 145e:** Ontology Based Decision Making for Process Control
- Bogdan Dorneanu, Mohamed
 Heshmat, Yang Gao, Harvey Arellano-Garcia
- 2:30 Paper 145f: Energy Harvesting Sensors Using Magnetic Phase Transition
- Yasuki Kansha, Masanori Ishizuka

(146) In Honor of Ruth Baltus I (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Barrel Spring I Jamie Hestekin, Chair Basavaraju Agasanapura, Co-Chair

Sponsored by: Membrane-Based Separations

- **12:30 Paper 146a:** Mechanisms of Improvements in Virus Control By Electrocoagulation: Removal and Inactivation
- Shankar Chellam
- 1:10 Paper 146b: Fabrication of Catalytic Water Treatment Membranes with Phosphorene-Based Pore Fillers — Phillip Mills, Joyner Eke, Isabel Escobar
- 1:32 Paper 146c: Tangential Flow for Analyte Capture (TFAC): A Method for the Purification of Nanoparticle Biomarkers Enabled By Ultrathin Silicon Membranes
- **James McGrath**, Kilean Lucas

- 1:54 Paper 146d: Understanding
 Fouling Mechanisms in Virus Filtration of
 Biotherapeutic Proteins
- **Christina Carbrello**, Benjamin Cacace, Sal Giglia
- **2:16** Paper 146e: Highly Selective Ultrafiltration Exploiting Non-Steric Interactions for Bioprocessing *Andrew L. Zydney*
- 2:38 Paper 146f: Additive Manufacturing of Thin Film Composite Membranes
- **Jeffrey R. McCutcheon**, Xin Qian, Tulasi Ravindran, Maqsud R. Chowdhury

(147) In Honor of the 2018 R.H. Wilhelm Award Winner I (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Florida Ballroom B

Stacey D. Finley, Chair David J. Klinke, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 147a:** A Graph-Theoretic Moiety Hypothesis for Olefin Yields from High Temperature Pyrolyses of C_8 to C_{12} Normal-, 2-Methyl- and 4-Methyl-Alkanes
- Preetinder S. Virk, Kevin Dahm
- **12:55** Paper **147b**: Software Tools for Molecular-Level Kinetic Modeling of Refinery and Petrochemical Reactors *Michael T. Klein*
- **1:20** Paper 147c: Reaction Engineering for Hydrothermal Conversion of Biomass *Phillip E. Savage*
- 1:45 Paper 147d: Catalyst Design and Production for Methane Dry Reforming Using a Flame-Driven High Temperature Reducing Jet Aerosol Reactor
- Mohammad Moein Mohammadi, Naveshkaanth Alexander, Anirudh Raghavan, William Sullivan, Raymond Buchner, Haiqing Lin, Carl R. F. Lund, Mark T. Swihart
- **2:10** Paper 147e: Extractable Content of Functional Acrylic Resins Produced By Radical Copolymerization: A Comparison of Experiment and Stochastic Simulation *Amin Nasresfahani, Loretta A.*
- Amin Nasresfahani, Loretta Idowu, Robin A. Hutchinson
- 2:35 Paper 147f: Identifying Promising Metal—Organic Frameworks for Methane Activation Via High-Throughput Periodic Density Functional Theory
- Andrew Rosen, Justin M. Notestein, Randall Q. Snurr

(148) Intellectual Property for Practicing Engineers: Patents and Trade Secrets

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom N

Sponsored by: Chemical Engineering & the Law Forum

12:30 Paper 148a: Asserting and Protecting IP Rights in Chemical and Pharmaceutical Industries

- Hana Oh

1:00 Paper 148b: Patents Are Integral to Monetizing Innovation. Court Decisions Have Led to Uncertainty As to What Is Patentable, Affecting Drug, Diagnostic, Genetic, and Other Innovation

- Matthew Zapadka

1:30 Paper 148c: Start-up, Spinout, Don't Burn-Out: Protecting Your Intellectual Assets on a Shoestring Budget

- Robert Sovesky

(149) Metabolic Engineering of Autotrophs

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 2 Nanette R. Boyle, Co-Chair Robert Jinkerson, Co-Chair Arul Varman, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 149a: Innovative Feedstock Design through Repartition of Photosynthetic Carbon to Terpene Production

— Joshua Yuan

12:48 Paper 149b: Synergistic Substrate Cofeeding Enables Rapid CO₂ to Product Conversion

— **Nian Liu**, Junyoung O. Park, Gregory Stephanopoulos

1:06 Paper **149c**: Improving Heterologous Protein Expression in *Synechocystis Sp. PCC 6803* for Alpha-Bisabolene Production

- Jacob Sebesta

1:24 Paper **149d:** Model-Guided Engineering of Cyanobacteria for Improved C₄-C₅ Alcohol Production — *Hugh M. Purdy, Jennifer L. Reed*

1:42 Paper 149e: Genome-Scale Metabolic Model of *Chromochloris*, an Emerging Model Organism for Sustainable Fuel Production

— Alexander Metcalf, Michelle Meagher, Anthony Nagygyor, Walter Prentice, Emily Bournia, Stuart Ramsey, Nanette R. Boyle

2:00 Paper 149f: Metabolic Reconstruction of Central Carbon Metabolism and Antioxidant Production in Microalgae: Modelling and Optimization

— **Safina Ujan**, Hector De la Hoz Siegler Jr.

2:18 Paper 149g: Biological Synthesis of Chemicals from ${\rm CO}_2$

— Shota Atsumi

(150) Modeling and Analysis of Chemical Reactors I: Steady-State Behavior

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom F Anthony G. Dixon, Chair Sarah Feicht, Co-Chair Justin A. Federici, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper **150a**: Modeling and Analysis of Instabilities in Autothermal Packed-Bed Catalytic Reactors

— Meet Shah, Balakotaiah Vemuri

12:50 Paper 150b: Microwave Heating of Packed Bed Reactors

— **Fanglin Che**, Himanshu Goyal, Dionisios G. Vlachos

1:10 Paper 150c: Application of Advanced Non-Invasive Radioisotope Techniques for Benchmarking and Scaling up of Multiphase Flow Reactors: Quantification and Validation of CFD

— Omar J. Farid, Binbin Qi, Muthanna H. Al-Dahhan

1:30 Paper 150d: Design of Membrane Reactor for Oxidative Coupling of Methane: Effects of Interphase Mass and Heat Transport Limitations

— **Ojotule P Onoja**, Panagiotis Kechagiopoulos

1:50 Paper 150e: Simulation of Commercial Scale Autothermal Chemical Looping Unit for Syngas Production

— **Zirui He**, Florent Minette, Juray De Wilde

2:10 Paper 150f: Modeling of NO_x reduction By Urea-Based Selective Catalytic Reduction in a Monolith Reactor

— **Niket S. Kaisare**, Preeti Aghalayam, Sruti Dammalapati, Risha Raju

2:30 Paper 150g: Trapping Properties of Ag/SSZ-13 Zeolite: Modeling Adsorption Capacity

— **Eric Walker**, Caitlin Horvatits, Dan Li, Michel Dupuis, Eleni A. Kyriakidou

(151) Nanobiotechnology for Sensors and Imaging II

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Discovery 46 Daniel Roxbury, Chair Margaret Bennewitz, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 151a: Carbon Nanotube Photoluminescence Solvatochromism in Biomedicine: Spectroscopy, Imaging, and Modulation

- Daniel Heller

1:00 Paper 151b: Xeno Nucleic Acid Nanosensors for Enhanced Stability — Alice J. Gillen, Justyna Kupis-Rozmysłowicz, Carlo Gigli, Nils

Schuergers, Ardemis A. Boghossian

1:18 Paper 151c: Sequence and Aggregation State Determine Stability, Endosomal Processing, and Long-Term Fate of DNA-Wrapped Carbon Nanotubes in Mammalian Cells — Mitchell Gravely, Mohammad

1:36 Paper 151d: Real-Time Detection of H₂O₂ Signaling in Wild-Type Plants with Nanobionics Approach

Moein Safaee, Daniel Roxbury

— Tedrick Thomas Salim Lew, Volodymyr Koman, Seon-Yeong Kwak, Kevin Silmore, Michael Strano

1:54 Paper 151e: Fluorescent Single-Walled Carbon Nanotubes for Protein Detection

- Gili Bisker

2:12 Paper 151f: Directed Evolution of the Optoelectronic Properties of Synthetic Nanomaterials

— **Benjamin Lambert**, Alice Gillen, Nils Schuergers, Shang-Jung Wu, Ardemis A. Boghossian

2:30 Paper 151g: The Impact of Covalent Functionalization on Single-Walled Carbon Nanotube Sensor Fluorescence and Function

— **Linda Chio**, Natalie Goh, Aishwarya Murali, Markita Landry

2:48 Paper 151h: Protein Corona Formation on Single-Walled Carbon Nanotubes for Applications in Biological Environments

— **Rebecca L. Pinals**, Markita Landry

(152) Nanotechnology and 3D Printing: The Intertwined Technologies

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Discovery 45 Chi-Hwa Wang, Chair Yan Yan Shery Huang, Co-Chair Pooya Davoodi, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 152a: Emerging Organ Models and Organ Printing for Regenerative Medicine

— Ali Khademhosseini

1:05 Paper 152b: 3D Layered Nano-Micro- Fibre Printing Techniques for Biological and Electronic Applications — *Yan Yan Shery Huang*

1:35 Paper 152c: Putting 3D Biofabrication to the Use of Tissue Model Fabrication

— Y. Shrike Zhang

2:05 Paper 152d: 3D Printing
Functional Voxels: Fate and Transport of
Quantum Dots Under Capillary Flow
— Katrina J. Donovan, James Stasiak,
Willie E. "Skip" Rochefort, Garry Hinch

2:23 Paper 152e: Radio Frequency and Microwave Heating of Preceramic Polymers and Its Application in Silicon Carbide Processing

— Nutan Patil, Mohammad Saed, Miladin Radovic, **Micah J. Green** 2:41 Paper 152f: Complex Multi-Layered Microparticle Laden Fixed Hydrogel Wound Dressing Fabricated Via 3D Printing for the Treatment of Thermal Burns

— **Jia Heng Teoh**, Anbu Mozhi Thamizhchelvan, Sook Muay Tay, Chi-Hwa Wang

(153) Novel and Unconventional Mixers

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 32 Aaron Strand, Chair Thomas A. Simpson, Co-Chair Sanja Miskovic, Co-Chair

Sponsored by: North American Mixing Forum

12:30 Paper **153a**: A Novel Approach to the Experimental Determination of *Njs* Using Electrical Resistance Tomography — *Baran Teoman*, *Piero M. Armenante*

12:51 Paper 153b: Characterization of Micromixing in a Rotor-Stator Spinning Disc Reactor: Effects of Gap Distance — Arturo N. Manzano Martinez, Melissa Assirelli, John van der Schaaf

1:12 Paper **153c:** (Micro-)Mixing Effect in Alkylbenzene Sulfonation Using Spinning Disc Technology

— **Roy van Kouwen**, Wyatt Winkenwerder, Sander Haase, Melissa Assirelli, Zach Brentzel, Bill Joyce, Tom Pagano, John van der Schaaf

1:33 Paper 153d: Intensification of Reaction-Diffusion Processes By Magnetic Nanomixing

— **Aleš Zadražil**, František Štěpánek, Dalimil Snita

1:54 Paper **153e**: Blending in Above Ground Storage Tanks with Side Entering Agitators: Effect of Scale and D/T

— **Jason J. Giacomelli**, Sarah J. Johnson, Richard K. Grenville

2:15 Paper 153f: Comparison of Power Consumption and Mixing Time of a Stirred Tank with Different Impellers
— Qinghua Zhang, Zhuotai Jia, Chao Yana, Zai-Sha Mao

2:36 Paper 153g: Characterization and Analysis of Mixing in a Soft-Elastic Reactor (SER)

— **Jie Xiao**, Minghui Liu, Chao Zou, Guillaume Delaplace, Romain Jeantet, Xiao Dong Chen

(154) NSF Workshop I: Highlights from CBET

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 29/30 Ram B. Gupta, Chair Richard Dickinson, Co-Chair

Sponsored by: Career Guidance Committee Liaison

12:30 Paper **154a**: Overview of Chemical, Bioengineering, Environmental, and Transport Systems Division (CBET)

— Richard Dickinson

- **12:55 Paper 154b:** Highlights of CBET Cluster on Chemical Process Systems
- Carole Read
- **1:15 Paper 154c:** Highlights of CBET Cluster on Engineering Biology and Health
- Steven Peretti
- **1:35 Paper 154d:** Highlights on CBET Cluster on Environmental Engineering & Sustainability
- Carl Rockne
- **1:55** Paper **154e**: Highlights of CBET Cluster on Transport Phenomena *William Olbricht*
- 2:15 Paper 154f: Interactive Question and Answer Session with NSF Program Directors
- **Richard Dickinson**, Carole Read, Steven Peretti, Carl Rockne, William Olbricht

(155) Phase Behavior and Flow of Reservoir Fluids

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Challenger 40 Nagasree Garapati, Chair Yingda Lu, Co-Chair

Sponsored by: Upstream Engineering and Flow Assurance Forum

- **12:30 Paper 155a:** Equilibrium and Non-Equilibrium Phase Behavior of CO₂ and Crude Oil Interactions
- Yuhao Yang, Xiaoli Li
- **12:50 Paper 155b:** Deciphering the Complex Fluid Phase Behavior in Nanoporous Materials
- **Gorakh Pawar**, Hai Huang, Michael P. Hoepfner
- 1:10 Paper 155c: Estimation of Three-Phase Relative Permeabilities for a Wag Process Using an Improved Ensemble Randomized Maximum Likelihood Algorithm
- Zhaoqi Fan
- **1:30 Paper 155d:** Measuring and Modelling Wax Deposit Kinetics in Thermally-Driven and Sloughing Regimes
- **Ghinwa Yaghy**, David Harbottle, Thibaut Charpentier, Lorenzo Fusi, Anne Neville
- **1:50 Paper 155e:** Use of Thermal Analysis and Rheometry to Study the Properties of Crude Oil
- Yash Adhia
- **2:10** Paper 155f: Asphaltene Destabilization Mechanism Investigated By Ultra-Small Angle X-Ray Scattering and *in Situ* Titration
- **Weiyi Kong**, Rizwanur Rahman, Josh Martineau, Yuan Yang, Mahmoud Elmehlawy, Brian Knapper, Michael P. Hoepfner

(156) Plenary: Topical Conference in Molecular and Materials Data Science Monday, Nov 11, 12:30 PM

Hyatt Regency Orlando, Peacock Spring
Jim Pfaendtner, Chair
Elizabeth Nance, Co-Chair
Johannes Hachmann, Co-Chair
Heather J. Kulik, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

- **12:30 Paper 156a:** Data Science for Assembly Engineering
- Sharon C. Glotzer
- **12:53 Paper 156b:** A Computational Roadmap for Better Electronic Noses
- Christopher E. Wilmer
- **1:08** Paper **156c:** Using Artificial Intelligence to Discover New Materials: The Role of Material Representations
- Christopher M. Wolverton
- 1:31 Paper 156d: CAR-Mediated T Cell Activation: Linking Molecularly-Detailed and Data-Driven Models
- Colin Cess, Jennifer A. Rohrs, **Stacey D. Finley**
- **1:46** Paper 156e: Data Enabled Discovery in Soft Materials Discovery *Juan J. DePablo*
- 2:09 Paper 156f: Combining Molecular Dynamics Simulations and Deep Learning to Predict Interfacial Properties — Reid C. Van Lehn, Atharva Kelkar, Bradley C. Dallin
- **2:24** Paper 156g: Artificial Intelligence in Materials Science: The Good, the Bad, and the Ugly
- Venkat Venkatasubramanian

(157) Process Innovations on Renewable Polymers and Biobased Intermediates

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 17 Yihui Tom Xu, Chair Danielle J. Mai, Co-Chair Shaibal Roy, Co-Chair

Sponsored by: Process Research and Innovation

- **12:30** Paper **157a**: A Novel Method of Producing 2,5-Diformylfuran at High Yields from Glucose
- **Ravikumar Gogar**, Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi
- **12:48** Paper **157b**: Bio-Based Benzoxazine Monomers and Polymers Based on Difuran Diamine (Dfda)
- **Mengwen Yu**, John La Scala, Giuseppe Palmese
- **1:06** Paper **157c**: Overcoming the Influence of HMF Reaction Mixture Constituents on Extraction Solvent Performance
- Andre De Haan

- 1:24 Paper 157d: The Chemical Properties Allowing the Tetrabutylphosphonium Chloride-Water Mixture to Efficiently Dissolve Cellulose in High Water Concentrations Via Molecular Dynamics
- Brad Crawford, Ahmed E. Ismail
- **1:42** Paper **157e:** Martini Coarse-Grained Model for Poly-e-Caprolactone in Acetone-Water Mixtures
- **Daniele Marchisio**, Alessio D. Lavino, Paola Carbone
- **2:00 Paper 157f:** Lignin-Based Functional Polymers
- Hailing Liu, Hoyong Chung
- 2:18 Paper 157g: Uncertainty and Sensitivity Analysis Assessing the Robustness of Models Employed in Superstructure Optimization for the Downstream Process Design of a Biorefinery
- **Nikolaus I. Vollmer**, Celina K. Yamakawa, Krist V. Gernaey, Solange I. Mussatto, Gürkan Sin
- **2:36** Paper 157h: Techno-Economic Analysis for Rapid Commercialization of Chitin Nanofiber Suspensions for Barrier Applications
- **Chinmay C. Satam**, Riley K. Geran, Cameron J. Coffey, Matthew J. Realff, J. Carson Meredith

(158) Quantitative Approaches to Disease Mechanisms and Therapies

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 14 David Rumschitzki, Co-Chair John Blazeck, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **12:30 Paper 158a:** Quantitative Imaging of Human Rhinovirus Gene Expression Kinetics at the Single-Cell Level
- Huicheng Shi, John Yin
- **12:48 Paper 158b:** CAM/Camkii Mediated Remodeling of PDZ Domains and the Inhibitory Influence of Syngap in the Post-Synaptic Density
- Patrick Giolando, **Barrett F. Davis**, Matthew Pharris, Tamara L. Kinzer-Ursem
- **1:06** Paper **158c:** A Mathematical Investigation of Chemotherapy-Induced Peripheral Neuropathy
- **Parul Verma**, Achim Kienle, Dietrich Flockerzi, Doraiswami Ramkrishna
- 1:24 Paper 158d: A Kinetic Model of Tumor-Induced Bone Disease Predicts Complex Response Dynamics to Bone-Specific Mechanical Forces and Drug Perturbations
- **Leonard A. Harris**, David Florian, Erik Beadle, Alyssa R. Merkel, Scott A. Guelcher, Julie A. Rhoades
- 1:42 Paper 158e: Characterizing the Role of Biomembrane Phase Separation in the Function and Regulation of the Drug Target Gamma-Secretal Williams Lovelings
- **M. Lane Gilchrist**, William Houlihan, Marilia Barros, Yueming Li

- 2:00 Paper 158f: Model-Based Diagnosis, Management, and Treatment of Chronic Obstructive Pulmonary Disease (COPD)
- **Navid Ghadipasha**, Anais Chalant, Bin Yu, Babatunde A. Ogunnaike
- 2:18 Paper 158g: Integrative Analysis of Free Fatty Acid-Induced NFkB Activation in Macrophages: A Step Towards the Quantitative Understanding of Inflammation Induced By Obesity

 Dongheon Lee, Yufang Ding, Arul Jayaraman, Joseph Sang-Il Kwon
- 2:36 Paper 158h: It Takes Two to Tango! Examples of Experiments/
 Simulations Combinations to Tackle Cancer Biology
- **Domenico Marson**, Andrea Mio, Erik Laurini, Suzana Aulic, Maurizio Fermeglia, Sabrina Pricl

(159) Reaction Chemistry and Engineering I: From Reaction Mechanisms to Continuous Synthesis

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom E Milad Abolhasani, Chair Hari Nair, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 159a:** Cooperative Activation of Cellulose with Alkaline Earth Metals
- **Gregory G. Facas**, Vineet Maliekkal, Matthew Neurock, Paul Dauenhauer
- **12:50 Paper 159b:** DFT and Micro-Kinetic Studies of Intermetallic Catalysts for Selective Hydrogenation
- **Haoran He**, Anish Dasgupta, Randall Meyer, Robert Rioux, Michael Janik
- **1:10** Paper **159c:** Convert Hydrogen Sulfide to Hydrogen By Iron Sulfide Via a Novel Thermo-Catalytic Sulfur Capture Process
- **Yu-Yen Chen**, Sourabh Nadgouda, Lang Qin, Kalyani Jangam, Liang-Shih Fan
- **1:30** Paper **159d**: Miniature CSTRs for the Synthesis of InP-Based Semiconductor Nanocrystals *loannis Lignos*, *Yiming Mo*, *Carayannopoulos Loukas*, *Klavs F*.
- **1:50 Paper 159e:** Assessment of Hazards for Green Oxidation of Secondary Alcohols with Hydrogen Peroxide
- Sun Yue, Lei Ni, Wen Zhu, Juncheng Jiang, M. Sam Mannan, Maria Papadaki, Benjamin A Wilhite
- **2:10** Paper 159f: Expert System for Automated Reaction Mechanism Generation
- **Udit Gupta**, Dionisios G. Vlachos

- 2:30 Paper 159g: Regioselectivity of Epoxide Ring Opening with Alcohols Using Lewis Acidic Zeolites and Nano-Zeolites
- **Nicholas Brunelli**, Nitish Deshpande, Aamena Parulkar, Rutuja Joshi, Ambarish Kulkarni

(160) Regenerative Engineering: Stem Cells and Mechanotransduction Monday, Nov 11, 12:30 PM

Hyatt Regency Orlando, Celebration 8 **Yusuf Khan, Chair**

Sponsored by: Regenerative Engineering Society

12:30 Paper 160a:Towards Regenerative Immunotherapy:
Using Biomaterials for Local Delivery

Bioactive Lipids and Pro-resolving
Lipid Mediators

Edward Botchwey

1:00 Paper 160b: The Effect of Centrifugal Force on the Mechanism of Wharton's Jelly Mesenchymal Stem Cells Transfection

— Leslie Vanessa Sánchez-Castillo, Andrés Arias-Arellano, Ana Isabel Ramos-Murillo, Gustavo Salguero López, Rubén D. Godoy-Silva

1:20 Paper 160c: Aggregation of Mesenchymal Stem Cells Rejuvenates Functionality Following *in Vitro* Aging through Induction of the Integrated Stress Response

— **Brent Bijonowski**, Qin Fu, Teng Ma

1:40 Paper 160d: Three-Dimensional Culture of Human Adipose-Derived Stem Cells By Surface Modification Using Elastin-Based Copolymers

- Sarah Fitzgerald, Amol V. Janorkar

2:00 Paper 160e: Delivering Therapeutic Drugs to Rejuvenate Progenitor Cells

— Donny Hanjaya-Putra

2:20 Paper 160f: Peptoid-Based Substrates for Human Neural Stem Cell Differentiation

— Shannon L. Servoss, **Joshua Corbitt**, Jesse Roberts, Ruben M. Ceballos

2:40 Paper 160g: Paper To Be Announced

(161) Software Engineering in and for the Molecular Sciences

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Rock Spring I/II Eric Jankowski, Chair

Sponsored by: Computational Molecular Science and Engineering Forum

12:30 Paper 161a: How to Professionally Develop Reusable Scientific Software – and When Not to

— **Carl Simon Adorf**, Vyas Ramasubramani, Joshua A. Anderson, Sharon C. Glotzer

12:45 Paper 161b: How to Design a Fast Nanocar

— **Kutay Berk Sezginel**, Jessica Nash, Christopher E. Wilmer 1:00 Paper 161c: Using Unified Memory and Nvlink for Node-Level Strong Scaling of Molecular Dynamics Simulations

— **Jens Glaser**, Peter Schwendeman, Joshua A. Anderson, Sharon C. Glotzer

1:15 Paper 161d: Efficient Trajectory Analysis Using Selection Tools in Gromacs

— **J. Patrick Brian**, Vance Jaeger

1:30 Paper 161e: Continuous Integration of Molecular Force Fields — Andreas Krämer, Martin Schenk, Robin Strickstrock, Richard W. Pastor, Karl N. Kirschner, Bernard R. Brooks, Dirk Reith

1:45 Paper 161f: A Software Module for Calculation of Virial Coefficients of Macromolecules

— **Arpit Bansal**, Andrew J. Schultz, David A. Kofke, Jack F. Douglas

2:00 Paper **161g**: A New Molecular Simulation Code Optimized for the State-of-the-Art Continuous Fractional Component Monte Carlo Method

- Remco Hens, Thijs J. H. Vlugt

2:15 Paper 161h: Gomc: GPU Optimized Monte Carlo for the Simulation of Phase Equilibria and Physical Properties of Complex Fluids

— Mohammad Barhaghi, Younes Nejahi, Gregory Schwing, Jason R. Mick, Brock Jackman, Kamel I. Rushaidat, Yuanzhe Li, Jeffrey J. Potoff, Loren Schwiebert

2:30 Paper 161i: Machine Learning for Molecular Property Predictions and the Software Ecosystem That Enables It

— Johannes Hachmann

2:45 Paper **161j**: Accelerating Large-Scale Screening of Tribological Properties and Chemistries

— **Justin Gilmer**, Andrew Z. Summers, Christopher R. lacovella, Peter T. Cummings, Clare McCabe

(162) Spotlights in Thermodynamics and Computational Molecular Science (Invited Talks)

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Silver Spring I/II

M. Scott Shell, Chair Coray M. Colina, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Introductory Remarks

12:35 Paper **162a**: The Outlook for Physically Informed Machine Learning in Computational Molecular Science

- Paulette Clancy

12:55 Paper 162b: Exploiting Electronic Structure and Machine Learning Models for Discovery in Transition Metal Chemistry

— **Heather J. Kulik**, Chenru Duan, Jon Paul Janet, Fang Liu, Aditya Nandy **1:15 Paper 162c:** Thermodynamic and Data-Centric Computational Methods to Guide Nanoparticle Design

— **Reid C. Van Lehn**, Bradley C. Dallin, Alex K. Chew, Atharva Kelkar

1:35 Paper **162d:** Self-Assembly of Complex and Universal Crystal Structures — *Julia Dshemuchadse*

1:55 Break

2:00 Paper 162e: Design of Components and Protocols for Inducing Protective Antibodies Against HIV

— Kayla Sprenger, Joy Louveau, Simone Conti, Victor Ovchinnikov, Martin Karplus, Arup K. Chakraborty

2:20 Paper 162f: Toward Engineering the Self-Assembly of Rigid-Soft Multiblock Oligomers

- Fernando A. Escobedo

2:40 Paper 162g: Molecular-Scale Experimental and Simulation Synergy to Improve Property Predictions

— **Michael P. Hoepfner**, Rizwanur Rahman, Mahmoud Elmehlawy, Abdur Rahman Shazed

(163) Student Paper Competition in Sensor Technology II

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 10 Qingshan Wei, Chair Ariel Furst, Co-Chair

Stephanie McCalla, Co-Chair

Sponsored by: Sensors

12:30 Paper 163a: Heavy Metal Detection and Biochemical Sensing Using Plant Nanobionics Approach — *Tedrick Thomas Salim Lew*,

Michael Strano

12:48 Paper **163b:** Electrochemical Point-of-Care Sensing Methods for the Detection of Tuberculosis Volatile Organic Biomarkers in Patient Breath and Condensate

— **Christina Willis**, Yalda Saffary, Anurag Tripathy, Manoranjan Misra, Swomitra Mohanty

1:06 Paper 163c: Reusable Electrochemical Cyclodextrin Biosensor for Resveratrol Detection

— **Zahra Panahi**, Jeffrey M. Halpern

1:24 Paper **163d:** Detecting Iron in Capillary Blood at the Point of Care with Colorimetric Sensing

— **Michael Serhan**, Mark Sprowls, Mindy Long, David Jackemeyer, Erica Forzani

1:42 Paper **163e**: Colorimetric Detection of Methicillin-Resistant *Staphylococcus Aureus* Using DNA Nano-Sensing Probes

— **Ymir Garcia**, Yu-Ching Tung, Hiroaki Sakamoto, Han-Sheng Chuang

2:00 Paper 163f: Developing Janus Particles Enabled Rotational Diffusometry for High-Sensitive Diabetic Retinopathy Detection

- Wei-Long Chen, Han-Sheng Chuang

2:18 Paper 163g: Early Screening of Infection Using Electrochemical Point-of-Care Biosensor

— **Ambalika S Tanak**, Sriram Muthukumar, Shalini Prasad

2:36 Paper 163h: Sensing Mechanisms of Floating Gate Transistors

— **Mathew Thomas**, Kevin D. Dorfman, C. Daniel Frisbie

(164) Sustainable Biorefineries Plenary Session (Invited Talks) Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Regency

Ballroom T Mark Mba Wright, Chair Fanxing Li, Co-Chair Peyman Fasahati, Co-Chair

Sponsored by: Sustainable Biorefineries

12:30 Paper 164a: Presentation Title TBD — *Lee R. Lynd*

12:55 Paper **164b**: Integrated Biorefinery Approach to Produce Biosugar from Lignocellulosic Biomass — *Sunkyu Park*

1:20 Paper 164c: Carboxylate Platform – Lessons from the Cow

— Mark Holtzapple

1:45 Paper 164d: Presentation Title TBD

— Tom L. Richard

2:10 Paper 164e: CELF Pretreatment of Cellulosic Biomass Achieves High Yields of Reactive Intermediates for Biological or Catalytic Conversion to Fuels and Chemicals

— Charles E. Wyman

(165) Career Paths: Perspectives by Minority Professionals in Chemical Engineering

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Regency Ballroom O Quinta Warren, Chair

Sipho C. Ndlela, Co-Chair Sponsored by: Minority Affairs

12:30 Introductory Remarks

12:32 Presentation by Harold Conner

12:52 Presentation by Quinta Warren

1:12 Panel Discussion

Committee (MAC)

2:58 Concluding Remarks

(166) Sustainable Management and Uses of Post-Consumer Materials and Waste

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Regency Ballroom U

Jason Trembly, Chair Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by: Sustainability Science and Engineering

- 12:30 Paper 166a: Understanding Formation of Nitrogen Heterocycles during Catalytic Hydrothermal Liquefaction
- Michael T. Timko, Richard H. West, Rasha Atwi
- 12:50 Paper 166b: Biochar and Activated Carbons Derived from Food Waste: Properties and Applications - Lei Yu, David P. Gamliel, Katherine M. Saltzgiver, Brianna Markunas, Julia
- 1:10 Paper 166c: A Framework for Assessing Solid Waste Energy Recovery Systems for Small-Scale on-Site Applications
- Andrew Pfluger, Pamela L. Sheehan, Enoch Nagelli, Corey James, Harry L. Moore, Preston Haney
- 1:30 Paper 166d: Microplastic Environmental Effect on the Aquatic Ecosystem of the Thermaic Gulf
- Marianthi Kermenidou, Irini Moschoula, Dimitris Kousis, Spyros Karakitsios, Dimosthenis Sarigiannis
- 1:50 Paper 166e: Study and Optimization of the Supply Chain of the Recollection and Harnessing of Used Cooking Oil in the City of Bogotá
- Juan Sebastián Rodríguez Flórez, Alvaro Orjuela
- 2:10 Paper 166f: Economic Feasibility of Evaporation-Based Liquid Digestate Treatment for Biogas Plants
- Michal Touš, Marek Vondra
- 2:30 Paper 166g: Strategies for Improvement of Anaerobic Digestion from Agricultural Waste: A Critical Review
- Safenaz Shaaban, Doaa Bassuney, **Mahmoud Nasr**
- (167) Synthesis and Application of Inorganic Materials: Part II Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Celebration 16 Mark Snyder, Chair

Sponsored by: Inorganic Materials

Aseem Chawla, Co-Chair

- 12:30 Paper 167a: Microwave-Initiated Synthesis of Metal Chalcogenides on Graphene for Energy Applications
- Shatila Sarwar, Xinyu Zhang, Amit Nautiyal, Jonathan Cook
- 12:48 Paper 167b: Synthesis of Nanoporous Metals through Thermal **Decomposition of Transition Metal** Dichalcogenides
- Swarnendu Chatterjee, Yawei Li, Saad Intikhab, Joshua Snyder
- 1:06 Paper 167c: Salt-Templated Metal and Metal Oxide Porous Materials - F. John Burpo, Enoch Nagelli, Anchor R. Losch, Jack Bui, Felita
- Zhang, Veronica Lucian, Brittany Aikin, Epiphanie Dongkeng
- 1:24 Paper 167d: Post-Synthetically Amine Grafted Silica Nanoparticles As Model Materials for Separations and Catalysis
- Peter Miller

- 1:42 Paper 167e: Using in-Situ Synchrotron Characterization Methods to Understand Structure/ Function Relationships for Catalytic Nanomaterials
- Nicholas Bedford
- 2:00 Paper 167f: Low-Cost Low-Temperature ALD of Titania Using Alkylamide Precursor and Oxygen with Urbach Tail Absorption in Visible Light Range for Potential Visible Light Adsorption
- Harshdeep Bhatia, Christos G. Takoudis
- 2:18 Paper 167g: Microporous-Mesoporous Hierarchical Structure for **Entrapping Functional Materials**
- Qiaobei Dong, Weiwei Xu, Fanglei Zhou, Ji Jiang, Dinesh Behera, Huazheng Li, Miao Yu
- 2:36 Paper 167h: Two-Dimensional Molybdenum Disulphide Membrane Separation: Stability, Structural Manipulation and Separation Performances — Shudong Jiang, Bingyi Guo**, Sui Z**hanq

(168) The Path Less Traveled: **Professional Development for Non-Tenure Track Faculty**

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 22 **Shannon Ciston, Chair** Stephen W. Thiel, Co-Chair

Sponsored by: Professional **Development Committee Liaison**

- 12:30 Paper 168a: Best Practices for **Teaching Focused Faculty**
- Tarvn Bayles
- 12:50 Paper 168b: Cultivating Support and Success As a Department's First Permanent Non-Tenure-Track Faculty
- Joshua A. Enszer
- 1:10 Paper 168c: Lessons from an Untenured Administrator...
- Daniel D. Burkey
- 1:30 Paper 168d: Presenting Yourself to the World: Academic Portfolio As a Professional Brand
- Sindia Rivera-Jimenez
- 1:50 Paper 168e: Panel Discussion: Getting Directions on the Path Less Traveled
- Shannon Ciston, Stephen W. Thiel

(169) Thermodynamic and Transport **Properties Under Pressure I**

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom K Erdogan Kiran, Chair Sabine Enders, Co-Chair

Sponsored by: High Pressure

- 12:30 Paper 169a: Modeling of n-Butane Solubility in Semi-Crystalline Polyethylene
- Sabine Enders, Michael **Fischlschweiger**

- 12:50 Paper 169b: The Effect of Solute-Solute Interactions in the Presence of CO₂ on the High Pressure Thermodynamic Behaviour of CO₂ + n-Alkane + 1-Alcohol Systems
- Cara E. Schwarz, Carla Latsky
- 1:10 Paper 169c: Estimation of Organic Solid Solute Solubility in the Supercritical Carbon Dioxide from Predictive Equations of State
- Zong-Zhe Cai**, Chieh-Ming Hsieh**
- 1:30 Paper 169d: Measurement of Diffusion Coefficient of Cr(acac)₃ in High Temperature Supercritical Carbon Dioxide — Toshitaka Funazukuri, Minoru
- Yamamoto, Junichi Sakabe, Chang Yi Kona
- 1:50 Paper 169e: High-Pressure Torsional Braid Analysis of Polymers in Carbon Dioxide: A New Twist in Polymer Characterization Under Pressure - Joseph Sarver, John C. Hassler,
- 2:10 Paper 169f: Hyperelastic Models for Studying Stress-Strain Curves of Processed Polymeric Systems with Supercritical CO, Techniques

Erdogan Kiran

- **Antonio Tabernero**, Lucia Baldino, Stefano Cardea, Eva M. Martín del Valle, Ernesto Reverchon
- 2:30 Paper 169g: Thermodynamic and Transport Data for Design of Processes with Sub-Critical and Super-Critical Fluids
- **Zeljko Knez**, Darija Cor, Zoran Novak, Milica Pantic, Gregor Kravanja, Masa Knez Hrncic

(170) Undergraduate Research Presentations - Energy and **Petrochemicals**

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 31 **Cory Thomas, Co-Chair**

Sponsored by: Young Professionals Committee (YPC)

(171) Getting Your Research Published (Invited Talks)

Monday, Nov 11, 1:30 PM Hyatt Regency Orlando, Rainbow Spring I/II

Arthur Baulch, Chair

Sponsored by: Publication Committee

(172) Wilson Award Winner (Invited Talks)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Discovery 43 **Thong Hang, Chair**

Sponsored by: Nuclear Engineering Division

(173) Negotiation and Evaluating a Job Offer for Nerds

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom L **April Grasso, Chair**

Sponsored by: Publication Committee

3:30 Paper 173a: Negotiation and Evaluating a Job Offer for Nerds - Alaina Levine

(174) General Poster Session I Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Sponsored by: Poster Sessions

Paper: Effects of Colloidal Network Characteristics on Crack Dynamics - Atiya Badar, Mahesh S. Tirumkudulu

Paper 755g: Cu- and Co-Based Catalysts for CO and C3H6 Oxidation in Diesel Exhaust

— **Zihao Li**, Yang Geng, Xiaoyin Chen, Johannes W. Schwank

Paper 174a: Electro-Plasmonic Neural Stimulation and Its Implication for Prosthetic Devices

- Ratka Damnjanovic, Parveen Bazard, Robert Frisina, Venkat R. Bhethanabotla

Paper 174b: Design of a Drug Delivery System Based on Levan-Capped Silver Nanoparticles for Bactericidal Purposes — Álvaro González-Garcinuño, Angel Dominguez, Rubén Masa, Maria Hernández, Eva M. Martín del Valle. Antonio Tabernero

Paper 174c: The Important Role That Size Plays into Polydopamine Nanoparticles' Antiproliferative Activity - Celia Nieto, Jesús Enrique, Milena Vega, Gema Marcelo, Miguel A. Galán, Eva M. Martín del Valle

Paper 174d: Polymeric Adsorbent for Lipopolysaccharides (LPS) Removal from **Biopharmaceutical Products**

- Sidharth Razdan, Sutapa Barua

Paper 174f: Thermo-Mechanical and Flow Properties of Polymer Nanocomposites

- Koteswararao Medidhi, Venkat Padmanabhan

Paper 174g: Interface of Ion-Containing Aqueous and Organic Phases within and out of Confinement

Monir Hosseini Anvari, Phillip Choi

Paper 174h: Mass-Based Finite Volume Scheme for Aggregation, Growth and Nucleation Population Balance Equation - **Mehakpreet Singh**, Hamza Ismail, Themis Matsoukas, Ahmad Albadarin, Gavin Walker

Paper 174i: Tribology of PVA Borax Gel on Silanized Silica

- Appu Vinod, Yagnavalkya Bhimayarapu, Rafael Tadmor, Semih Gulec. Sakshi Yadav

Paper 174j: Scale-up of Stirred Tanks Applied to Newtonian Liquids Daniel Torneiros, Murilo Lucindo, Marlene Moraes, Aldo Santos, Deovaldo Moraes Júnior, Vitor Rosa

Paper 174k: Unidirectional Large-Amplitude Oscillaltory Shear FLOW of Blood - Chaimongkol Saengow, A. Jeffrey Giacomin, Andrea Dimitrov

Paper 1741: Synthesis and Identification of Modified Magnetic Carbon Nanoparticle and Study of Its Application in Removing Lead Ions (Pb²*) from Aqueous Solution

— Bizhan Honarvar

Paper 174m: Aluminum Thin Film Enhanced Native Fluorescence for Biosensors in the UV Spectral Region — Ji-Young Lee, Yunshan Wanq

Paper 174n: Engineering Colloidal Templates for Tuning Nanoparticle Surface Interactions and Optical Responses

— Alice J. Gillen, Daniel J. Siefman, Shang-Jung Wu, Benjamin Lambert, Ardemis A. Boghossian

Paper 174o: Evolution of Magnetic Properties, Heating Rate, and Mpi Performance of Iron Oxide Nanoparticles during Post-Synthesis Oxidation

— **Sitong Liu**, Shehaab Savliwala, Carlos Rinaldi

Paper 174p: Nanostructure Control of Biosensing Materials: From Fundamental Research to Industrial Instrument

— **Zhenyu Chu**, Wangin Jin

 $\begin{array}{l} \textbf{Paper 174q:} \ \textbf{Amino Acid Coated Coated} \\ \textbf{Gd}_2\textbf{O}_3 \ \textbf{Nanoparticles As a Potential} \\ \textbf{T}_2 \ \textbf{MRI-CT Dual Contrast Agents} \end{array}$

— **Mohammad Ahmad**, Mazhar Ul Islam

Paper 174r: A Computationally Efficient Procedure for Studying Segregation in Alloy Materials with Monte Carlo Simulations

— **Gargi Agrahari**, Abhijit Chatterjee

Paper 174s: How to Model Local Solvation Environments in Pure Liquids and Complicated Mixtures without Dynamics

- Yasemin Basdogan, John A. Keith

Paper 174u: Understanding Binding Behavior in Host-Guest Systems Using Advanced Sampling Simulations — Anne C. Leonhard, Jonathan K.

Whitmer

Paper 174v: Development of Transferable Coarse-Grained Models of Amino Acids

— Olivia Conway, Yaxin An, Karteek K. Bejagam**, Sanket A. Deshmukh**

Paper 174w: Study of MOF-Polymer Compatibility Using Molecular Dynamics Simulations

— **Abhishek Sose**, Samrendra Singh, Karteek K. Bejagam, Sanket A. Deshmukh

Paper 174x: Entropic Contributions to Supramolecular Assembly of Liquid Hydrocarbons

— **Rizwanur Rahman**, Yuan Yang, Thomas Headen, Michael P. Hoepfner

Paper 174z: Experimental Proof-of Concept and Model-Based Analysis of an Autonomous Sabatier Reactor for Thermocatalytic Conversion of CO₂

— Yichen Zhuang, **David Simakov**

Paper 174aa: Cooling and Dilution Effects in a Thermally Integrated Microreactor for Sabatier Reaction

— **Aswathy K. Raghu**, Niket S. Kaisare

Paper 174ab: Quantification and Pseudo-3D Modelling of Liquid Holdup and Maldistribution in a Trickle Bed Reactor with Validation Using Gamma-Ray Computed Tomography

— Binbin Qi, Omar J. Farid, Muthanna H. Al-Dahhan

Paper 174ac: An Approach for Methanol-to-Olefin (MTO) Reaction Kinetics Using Simple but Efficient Lumped Model

— Min-kyung Lee, **Jun-Hyung Ryu**, In-Beum Lee

Paper 174ad: Functionalizing Cell Membrane with a Multifunctional DNA-Origami Platform for Biomulecular Detection

— **Melika Shahhosseini**, Ehsan Akbari, Jonathan W. Song, Carlos E. Castro

Paper 174af: Curvature-Driven Adsorption and Alignment of Cationic Nanoparticles to Phase Boundaries in Multicomponent Lipid Bilayers

— **Jonathan K. Sheavly**, Reid C. Van Lehn

Paper 174ag: Study the Diffusion Mechanism and Diffusivity of Lithium Ions in the Ionic-Liquids-Added Electrolytes Using Molecular Simulation — Qiang Wu, Nan Xu, Yao Shi, Yi He

Paper 174ai: Crude Oil Spot Sampling Methods and Their Impact on Thermophysical Properties

— **Joseph W. Hogge**, David L. Lord, Raymond Allen, David K. Rudeen

Paper 174aj: Continuous Flow Synthesis of Energetic Materials

— Eric Gauthier

Paper 174ak: Mechanisms of Xylene Isomer Oxidation By Non-Thermal Plasma Via Paired Experiments and Simulations

— Tianyu Shou, Nan Xu, Yao Shi, Yi He

Paper 174al: Pleiotropic Effect of Glycan Perturbation on Leukocyte Immunological Response

— **Xinheng Yu**, Theodore Groth, Panagiotis Mistriotis, Alexandros Afthinos, Konstantinos Konstantopoulos, Sriram Neelamegham

Paper 174am: Development of Novel Stability Assays for Protein Biopharmaceuticals Using Time-Dependent Light Scattering Analysis

— **Cathryn Conner**, James McAndrew, Stefano Menegatti, Orlin D. Velev

Paper 174an: A Novel Ni@Zn-MOF Catalyst Activated Persulphate System for the Efficient Degradation of Orange II

— **Muhammad Danish**, Usman Farooq, Sajjad Ahmad, Syed Waqas Ahmad, Ayyaz Ahmad

Paper 174ao: Hybrid Liquid Membrane Method for Removal of Arsenic from Drinking Water

— Soumi Sarkar, Prabirkumar Saha

Paper 174ap: Supported Liquid Membranes for π Electron Induced Fractionation and Separation of Aromatics and Stereoisomers

— **Mohanad Kamaz**, Arijit Sengupta, Xianghong Qian, Ranil Wickramasinghe

Paper 174aq: Role of Multi-Walled Carbon Nanotubes in Improving Flux and Antifouling Property of Polyethersulfone Hollow Fiber Membrane

— **Preety Kumari**, Akshay Modi, Jayesh R. Bellare

Paper 174at: Butyl Acetate Recovery in Dilute Aqueous Solution Via Sn-Silicalite-1 Membrane Pervaporation

— **Kun Liang Ang**, Eng Toon Saw, Xuecheng Dong, Wei He, Seeram Ramakrishna

Paper 174au: Optimization of Chondrogenic Differentiation of Adipose-Derived Stem Cells through Co-Culture with Chondrocytes and Addition of Growth Factor and Nutraceutical Compounds

— Olivia Reynolds, Haneen Abusharkh, Nehal I. Abu-Lail, Arda Gozen, Juana Mendenhall, Bernard J. Van Wie

Paper 174av: Towards Identification of Critical Quality Attributes of Chondrogenic Microtissues-a Metabolomics Perspective

— **Niki Loverdou**, Gabriella Nilsson Hall, Kristel Bernaerts, Bart Ghesquière, Geert Carmeliet, Ioannis Papantoniou, Liesbet Geris

Paper 174ax: Investigating the 3-D Assembly of Chemically Specific Building Blocks for Covalent Organic Frameworks

— **Tiara Maula**, Srinivas Rangarajan, Jeetain Mittal

Paper 174ay: Ensemble-Based Machine Learning for Industrial Fermenter Classification and Foaming Control — Aman Agarwal, Y.A. Liu, Christopher

McDowell
Paper 174az: Determination and

Paper 174az: Determination and Modelling of the Reciprocal Quaternary Solid-Liquid Phase Equilibrium for the Systems K+,NH₄+//Cl-,H₂PO₄--H₂O at 283.15K

— Qiang Wu, Xue Hu, Jing Zhu, **Tianxiang Li**

Paper 174bb: Time-Dependent FTIR Microscopy for Mechanism Investigations and Kinetic Measurements in Interfacial Polymerisation: A Microporous Polymer Nanofilm Study

— Dan Ren

Paper 174bc: PAT-Facilitated Crystallization Development and Particle Engineering Via Mechanistic Understanding

— Juana Du, Peter Fung, Alex Goldberg, **Chiajen Lai**, Helen Mah, Curtis Rieder, HoYan Sun, Joey Su Paper 174bd: Modeling of Cation Exchange Membranes Using Maxwell-Stefan Approach for Chlor-Alkali System — Ria Sijabat, Thijs de Groot, John van der Schaaf

Paper 174be: Two-Membrane Air Fresheners for Enhanced Non-Energized Perfume Delivery

— **Gui Min Shi**, Bee Ting Low, Kelly Anderson, Neal Tai-Shung Chung

Paper 174bg: High-Performance TFC
Membranes with Optimized Polyamide
Selective Layer for Water Treatment
— Shu Xiong, Liang Shen, Yan Wang

Paper 174bi: Atomic Layer Deposition-Enabled Conversion of Porous Polyethersulphone to Laser-Induced Graphene for Charged Membrane

Applications
— **David S. Bergsman**, Bezawit A.
Getachew, Jeffrey C. Grossman

Paper 174bj: Synthesizing Temperature Control System for Binary Distillation Columns

— **Lu Liu**, Kejin Huang, Yang Yuan, Xing Qian, Haisheng Chen, Liang Zhang, Shaofeng Wang

Paper 174bk: Revisit the Molecular Sieving Behavior in Zeolite LTA for High-Performance Gas Separation

- Jin Shang

Paper 174bm: Experimental Study of Cation Exchange Membrane Performance in Intensified Chlor-Alkali Electrolysis

— **Ria Sijabat**, Thijs de Groot, John van der Schaaf

Paper 174bn: Preventing "Crusty" Phase Impurities during Crystallization Scale-up

- Kathryn Meintel

Paper 174bo: Maxwell-Stefan Modeling and Experimental Study on the Ionic Resistance of Nafion 117

— **Ria Sijabat**, Thijs de Groot, John van der Schaaf

Paper 174bp: Dielectrophoresis-Based Motion for Switching of Microparticles: Numerical Modeling and Experimentation

— **Waqas Waheed**, Anas Alazzam, Bobby Mathew, Ashraf N. Al-Khateeb, Eiyad Abu Nada

Paper 174br: Efficient Degradation of Imidacloprid through Biochar Activated Sodium Percarbonate

— **Muhammad Danish**, Usman Farooq, Sajjad Ahmad, Syed Waqas Ahmad, Ayyaz Ahmad, Shuguang Lu

Paper 174bs: A Novel Hollow Fiber Membrane Embedded Co-Axial Microdevice for Simultaneous Extraction and Stripping

— Zifei Yan

Paper 174bt: Efficient Degradation of Norfloxacin By Zeolite Supported Zero-Valent Iron Activated Peroxydisulfate: Performance, Toxicity, Intermediates and Mechanism

— **Muhammad Danish**, Usman Farooq, Sajjad Ahmad, Syed Waqas Ahmad, Ayyaz Ahmad

Paper 174bu: Amphibians-Inspired Amino Acid Ionic Liquid Functionalized Nanofiltration Membranes with High Flux and Ion Selectivity for Wastewater Treatment

— **Hui-Fang Xiao**, Chang-Hui Chu, Shi-Peng Sun

Paper 174bv: Photon Upconversion for Real World Applications

- Daniel Congreve

Paper 174bw: Sustainable, Efficient, and Robust Mxene-Based Emulsion Liquid Membranes for Heavy Metals Removal

— **Saeed Laki**, Ahmad Arabi Shamsabadi, Farbod Alimohammadi, Babak Anasori, Masoud Soroush

Paper 174bx: Colloidal ReO₃ Nanocrystals: Extra Rhenium d-Electron Instigating a Plasmonic Response

— Sandeep Ghosh, Delia J. Milliron

Paper 174by: Wnt-Notch Signaling Interactions during Neural and Glial Patterning of Human Induced Pluripotent Stem Cells

— **Julie Bejoy**, Yan Li, Teng Ma

Paper 174bz: High Throughput Embryotoxicity Assay of Drugs and Chemicals Based on Embryonic Stem Cell-EGFP Reporter System

— **Fengli Zhang**, Ru Zang, Shang-Tian Yang

Paper 174ca: Site-Specific Covalent Immobilization of β-Agarase Onto Magnetic Nanoparticles for the Conversion of *Gelidium Amansii* into Biologically-Active Sugars

— Teklebrahan G. K. Weldemhret, Grace M. Nisola, Kristine Rose M. Ramos, Kris Niño G. Valdehuesa, Won-Keun Lee, Wook-Jin Chung

Paper 174cb: Maleic Anhydride Vapor Diffusion in Nafion Membranes

— Subasri Ayyadurai, Junchuan Fang, Jonathan Nickels**, Anastasios Anaelopoulos**

Paper 174cc: Monoethanolamine Based DES for CO₂ Absorption: Insights from Molecular Dynamics Simulations

— **Dina Kussainova**, Dhawal Shah

Paper 174cd: Harmful Components Migration and Transformation in the Chemical Looping Gasification of Phosphogypsum As Oxygen Carrier

— Liping Ma

Paper 174ce: Synergistic Enhancement of CO₂ Adsorption Rate and Capacity in Polyamine-Based Protic Ionic Liquids Functionalized Highly Ordered Mesoporous Silica

— Wei Zhang, Yao Shi, Yi He

Paper 174cf: Reaction Kinetics of Carbon Dioxide with Aqueous Solution of DEEP Eutectic Solvent & Methyl Diethanolamine Amine Using the Stopped Flow Technique

— **Hani Ababneh**, Abdelbaki Benamor, Mustafa Nasser, Muftah El-Naas

Paper 174cg: The Self-Reactivation
Performance of Nano-CaO-Based CO₂
Adsorbents in Calcium Looping Process
— Hao Liu, Sufang Wu

Paper 174ch: Biosensor Enabled Microbial Strain Improvement for Bioplastics Manufacturing

— Niju Narayanan

(175) Poster Session: Bioengineering Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

Nicholas R. Sandoval, Chair J. Andrew Jones, Co-Chair Jason T. Boock, Co-Chair Ryan M. Summers, Co-Chair Aditya M. Kunjapur, Co-Chair Arul Varman, Co-Chair

Sponsored by: Bioengineering

■ SYNTHETIC BIOLOGY

Paper 175a: Fine-Tuning Expression of Genes in *E. coli* Using a Theophylline-Sensing Hammerhead Riboswitch

— **Alexandra Wrist**, Ryan M. Summers

Paper 175b: Programming Animal Lipid Metabolism through Engineered Bacteria

— Baizhen Gao, Qing Sun

Paper 175c: Development of a Cripsr/ Cas_g-Based Recombineering System for the Genome Editing of Rhodococcus

— **Youxiang Liang**, Song Jiao, Huimin Yu, Zhongyao Shen

Paper 175d: GT DNA Assembly Standard

— **Xiaoqiang Ma**, Xiaoyi Cui, Hong Liang, Yurou Liu, Hongyuan Lu, Wenbo Ning, Nga Yu Poon, Kang Zhou

Paper 175e: Development of Toxr-like pH Regulator for the Optimization of Dahms Pathway in Engineered Escherichia coli

— Angelo B. Bañares, Kristine Rose M. Ramos, Won-Keun Lee, Grace M. Nisola, Kris Niño G. Valdehuesa, Wook-Jin Chuna

Paper 175f: Generalizing Noise Decomposition to Elucidate Nonlinear Gene Expression Noise

— **Tyler Quarton**, Leonidas Bleris

Paper 382c: Protein Structure Prediction and Design in a Biologically-Realistic Implicit Membrane

— **Rebecca F. Alford**, Patrick Fleming, Karen G. Fleming, Jeffrey J. Gray

■ BIOCATALYSTS & BIO-BASED PRODUCTS AND MATERIALS

Paper 175g: Effect of Spectral Down Conversion on Growth of Microalgae in a Photobioreactor

— **Indreesh Badrinarayanan**, Daniel W. Crunkleton, Tyler Johannes

Paper 175h: High Production of Butyric Acid through Simultaneous Utilization of Mannitol and Sugars from Macroalgae and Rice Straw

— **Youngsoon Um**, Hyun Ju Oh, Sun-Mi Lee, Gyeongtaek Gong, Min-Kyu Oh

Paper 175j: Cellulase Adsorption on Sugarcane Bagasse Lignin at 30 and 45°C

— Antonio C. F. dos Santos, Ariane Zanchetta, Eduardo Ximenes, Christiane C.C. Nunes, Mauricio Boscolo, Eleni Gomes, Michael R. Ladisch

Paper 175k: Growth Kinetics and Thermal Characterization of *Neochloris Oleoabundans* for Biofuel Production — Shaikh Razzak

Paper 1751: Subcritical aqueous phase oxidation of the waste generated from alkaline pretreatment of lignocellulosic biomass

— Vinod S. Amar, Anuj Thakkar, Bharat Maddipudi, Sandeep Kumar, Rajesh Shende

Paper 175m: Development of Artificial Garlic Cell with Potent in Vitro Bactericidal Effect

— **Petra Janska**, Viola Tokarova, Ondřej Kašpar, František Štěpánek

Paper 175n: Mechanisms of Microbially Influenced Corrosion Enabled By Acidithiobacillus Ferrooxidans

— **Yuta Inaba**, Alan C. West, Scott Banta

■ CELL CULTURE ENGINEERING

Paper 175o: Emerging Role of Polycyclic Aromatic Hydrocarbons (PAHs) in the Development of Adverse Outcome Pathways (AOPs) Linking Human Exposure and Health Outcomes

— **Ilias Frydas**, Spyros Karakitsios, Dimosthenis Sarigiannis

Paper 175p: Engineering and Characterization of Human Stem Cell-Derived Multicellular Aggregates of Glial Cells

— **Kyle Griffin**, Julie Bejoy, Liqing Sonq, Yan Li

Paper 175q: Evaluation of Commercial Media and Feed for Improved Mab Production

— **Baohua Zhang**, Ligang Zhou, Namratha Kuloor, Amlan Das

Paper 175r: Collagen – Poly (Ethylene Glycol) Hydrogel Matrix Modulation for Cancer Self-Organization

— **Kathryn M. Sullivan**, John D. Ito, William Ballance, Mikhail Kandel, Byoungsoo Kim, Gabriel Popescu, Hyunjoon Konq

Paper 175s: Comparison of Metabolic Gene Expression Levels between Lactate-Consuming and Lactate-Producing CHO Cell Cultures

— George Chacko

Paper 175t: Utilizing CRISPR-Cas₉ Genome Editing of Transcription Factors to Improve the Homogeneity of Neural Stem Cell Differentiation for Cell-Based Therapies

— **Kevin Chen**, S. Patrick Walton, Christina Chan

Paper 175u: Salinomycin Modulates Antitumor Immune Response By Repolarized Tumor-Associated Macrophages Toward M, Phenotype — Hugn Shen

Paper 175v: Comparison of CHO Cell Cultures Performance in Shaken and Spinner Flasks Bioreactors at the Same Value of Volumetric Mass Transfer Coefficient

— Andrés Javier Bello-Hernández, Rubén Darío Godoy-Silva

Paper 175bb: Model-Based Design of Non-affinity Chromatofocusing Capture Method for On-demand Production of Biologics

— **Sevda Deldari**, Payam Rezaei, Yang Liu, Abhay Andar, Govind Rao, Douglas D. Frey

■ METABOLIC ENGINEERING

Paper 175w: Biotransformation of Lignin Derived Aromatics through Metabolic Engineering of Corynebacterium Glutamicum for Flavonoid Production — Carlie L. Rein, Adam Wong, Michael Machas, David R. Nielsen, Arul M. Varman

Paper 175x: *De Novo* Production of a Biodegradable Solvent in *Escherichia coli* via Metabolic Engineering

— Aditya Sarnaik, Amit Kumar Jha, Abigail Jansen, Kunjkumar Patel, Ryan Davis, Arul Varman

Paper 175y: Engineering Bacillus Subtillis for the Secretion of Hydrolases Towards Consolidated Bioprocessing of Cellulosic Biomass

— **Apurv Mhatre**, Zachary Rudebeck, Arul Varman

Paper 175z: Efficient Biological Activation and Conversion of Short-Chain Hydrocarbons

— **Seung Hwan Lee**, James M. Clomburg, Patrick C. Cirino, Ramon Gonzalez

Paper 175aa: Constructing Ethanol Utilization Pathway (EUP) in *Escherichia*

— **Hong Liang**, Xiaoqiang Ma, Yurou Liu, Wenbo Ning, Anthony J. Sinskey, Gregory Stephanopoulos, Kang Zhou

Paper 175ab: Optimizing Cellobiose Consumption of Escherichia coli by Metabolic Engineering and Adaptive Laboratory Evolution

— Kris Niño G. Valdehuesa, Angelo B. Bañares, Grace M. Nisola, Won-Keun Lee, Wook-Jin Chung

Paper 175ac: Characterization of the Transcription Regulators Cafr and Caft from *Pseudomonas Putida* CBB₅
— *Shelby Brooks*, *Ward Pullen*, *Chris*

Raddatz, Ryan M. Summers

Paper 175ad: N-Butanol Production from Lignocellulosic Biomass By Engineered Clostridium Cellulovorans — Teng Bao, Wenjie Hou, Shang-Tian Yang

Paper 175ae: Establishing Probiotic Saccharomyces Boulardii As a Model Organism for Synthesis and Delivery of Biomolecules to the Mammalian Gut

— Ibrahim Al'Abri

Paper 175af: Continuous Production of 1.3-Propanediol By Metabolically Engineered Cyanobacteria Employing an Airlift Photobioreactor with pH-Stat System

— **Jun-ichi Horiuchi**, Yoichi Kumada, Taizo Hanai, Yasutaka Hirokawa, Akio Murakami, Mayuko Takeda

COMPUTATIONAL MODELING AND DOWNSTREAM PROCESSING

Paper 175ah: Modeling of Notch and PU₁ Regulation in T-Cell Vs Myeloid Differentiation

— **Shakti Gupta**, Merril Gersten, Neil Kumar, Shankar Subramaniam

Paper 175ai: Computational Analysis of Xylitol Production in Candida Tropicalis — Diana C. Tusso, Oscar Dias, Andrés Mauricio Pinzon Velasco, Mario Enrique Velásquez Lozano, Isabel Rocha

Paper 175aj: Enhancing Separation of Monomer and Aggregate with Mobile Phase Modifiers in Mixed Mode Chromatography

— Frank Bartnik, Timothy Pabst

Paper 175ak: Therapeutic Applications of an Algorithm for Ultra-Rapid Binding Interaction Engineering

— **Ritankar Bhattacharya**, Varun Chauhan, Robert Pantazes

Paper 175al: Genome-Scale Model Reconstruction and Application for the Non-Model Oleaginous Yeast *Rhodosporidium Toruloides*

— **Hoang V. Dinh**, Patrick F. Suthers, Siu Hung Joshua Chan, Yihui Shen, Tianxia Xiao, Anshu Deewan, Sujit Jagtap, Huimin Zhao, Christopher V. Rao, Joshua D. Rabinowitz, Costas D. Maranas

Paper 175am: Macroscopic Modeling of Bioreactors for Recombinant Protein Producing *Pichia Pastoris* in Defined Medium

— **Moo Sun Hong**, M. Lourdes Velez-Suberbie, Andrew J. Maloney, Andrew Biedermann, Kerry Routenberg Love, J. Christopher Love, Tarit K. Mukhopadhyay, Richard D. Braatz

Paper 175ao: Kinetics Study of CHO Cell
— Wanyue Cui, Shijie Liu

PROTEIN SCIENCE AND ENGINEERING

Paper 175ap: Optimizing Bias for Activation of Tumor-Reactive T Cell Subsets

— **Elissa Leonard**, Jamie B. Spangler

Paper 175aq: Immunoengineered Therapeutic Platform for Selective Immune Cell Activation

- Derek VanDyke, Jamie B. Spangler

Paper 175ar: An Innovative Method for the Characterization of Multi-Substrate Enzyme Reactions

— Thomas Waluga, Yasemin Kraus, Anna Krüger**, Jens Johannsen**

NOVEL DEVICES AND BIONANOTECHNOLOGY

Paper 175as: Polyanhydride Nanoparticle Encapsulation Preserves Stability and Antigenicity of Mucin-Based Antigen upon Release

— Luman Liu, Prakash Kshirsagar, John Christiansen, Shailendra Gautam, Sushil Kumar, Joyce Solheim, Surinder Batra, Maneesh Jain, Michael Wannemuehler, Balaji Narasimhan

Paper 175at: A Triple-Input Microfluidic Droplet Trapping Array for Multiplexed Single Cell Analysis

— **Khashayar R. Bajgiran**, Riad Elkhanoufi, James A. Dorman, Adam T. Melvin

Paper 175au: Tumor-Targeted Miniature Device for Bioimpedance Measurement and Treatment

- Ai Lin Chin, Rong Tong

Paper 175av: Biosynthetic Conversion of Ag+ to Ag₀ Nanoparticles By *Chlamydo-monas Reinhardtii*: Effects of Extracellular Polymeric Substance and Cell Components on Synthesis & Stability

— **Ashiqur Rahman**, Shishir V Kumar, Adarsh Bafana, Si Amar Dahoumane, Clayton Jeffryes

Paper 175aw: Algae Species on Turf Filter Reactor for Space Explorations

— **Remil Aguda**, Brandon LeBlanc, Cody Stelly, William Holmes, Rafael Hernandez, Mark Zappi, Emmanuel Revellame

Paper 175ax: Biofilm Removal Using Reversible Shape Memory Polymer — Sang Won Lee, Ivan Gitsov Ivanov, Dacheng Ren

Paper 175ay: Utilizing Gold Nanoparticles and Osmolytes to Detect Virus Particles Non-Specifically

— **Dylan G. Turpeinen**, Xue Mi, Ellie Lucier, Seth Kriz, James Chen Yong Kah, Carvn L. Heldt

Paper 175az: Nano-Immunosensors for Rapid Detection of Foodborne Toxin — *Huipin Cheng, Han-Sheng Chuang*

Paper 175ba: From Cell Pairs to Tissue Chips: Multi-Scale In Vitro Models for Screening Engineered Nanomaterial Toxicity

— Herdeline Ann M. Ardoña, John Zimmerman, Feyisayo Eweje, Seungkuk Ahn, Blakely O'Connor, Thomas Grevesse, Johan U. Lind, Kevin Kit Parker (176) Poster Session: Engineering Fundamentals in Life Science Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S Stacey D. Finley, Chair Michael Gower, Co-Chair Whitney L. Stoppel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

Paper 176a: A New Strategy for Identification of DNA Zip Codes Via Targeted Rewiring of Endogenous Loci in Mammalian Cells

— Meng Zhang

Paper 176b: Ipro+/-: A Computational Protein Design Tool Allowing NOT ONLY for Amino Acid Changes but Also Insertions and Deletions

- Ratul Chowdhury, Costas Maranas

Paper 176c: Modulation of Mitochondrial Activity in Human Mesenchymal Stem Cells with Biomolecules to Maintain Cell Stemness

— Kara Poole, Abigail Jones, Andrea Jimenez-Vergara, Lindsey Lubianski, Michael Garcia, Kwan Cheng, Dany Munoz-Pinto

Paper 176d: Simple and Efficient Gene Knock-in Strategy in Human Cell Lines Using 5' Modified dsDNA Donors with Short Homology Arms

— Qiqi Tian

Paper 176e: Post-Processing of 3D Bioprinted Human Dermal Tissue in the Dynamic Culture Environment of a Taylor-Couette Device

— **Jia Heng Teoh**, Anbu Mozhi Thamizhchelvan, Chi-Hwa Wang

Paper 176f: Transplantation of 3D Human Mesenchymal Stem Cell Aggregates As Regeneration Centers for Ischemic Stroke Treatment

— **Xuegang Yuan**, Shannon Helsper, F. Andrew Bagdasarian, Jens T. Rosenberg, Samuel C. Grant, Teng Ma

Paper 176g: 3D Dynamic Culture Enhances Extracellular Vesicle Production with Altered Biogenesis and Cargo Contents in Human Mesenchymal Stem Cells

— **Xuegang Yuan**, Dingani Nkosi, Qin Fu, Yuan Liu, Richard Jeske, Li Sun, David Meckes, Teng Ma

Paper 176h: Proteomic Analysis Reveals the Key Role of Integrated Stress Response in Restoring the Stemness of Culture Expanded Mesenchymal Stem Cells in 3D Aggregates

— Qin Fu, Brent Bijonowski, Xuegang Yuan, Yuan Liu, Richard Jeske, Teng Ma

Paper 176i: Differentiating Human Pluripotent Stem Cells into Vascular Smooth Muscle Cells in Three Dimensional Thermoreversible Hydrogels

— **Ou Wang**, Haishuang Lin, Qiang Li, Qian Du, Bin Duan, Yuguo Leo Lei, Chi Zhang Paper 176j: 3D Migration of Fibroblast-Macrophage Co-Cultures in Mechanically-Gradient Collagen Hydrogels

— **Rosalyn Hatlen**, Padmavathy Rajagopalan

Paper 176k: Closer to Reality: Development of Biocompatible Hydrogels to Validate Antitumor Activity and Specificity of a New Targeted paclitaxel Nanovehicle through 3D Cell Cultures

— **Celia Nieto**, Patricia Pérez-Esteban, Ivan Wall, Miguel A. Galán, Eva M. Martín del Valle

Paper 1761: Manufacturing Human Pluripotent Stem Cell Derived Endothelial Cells in Scalable and Cell-Friendly Microenvironments

— **Ou Wang**, Haishuang Lin, Qiang Li, Qian Du, Chi Zhang, Bin Duan, Yuguo Leo Lei

Paper 176m: A Scalable and Efficient Bioprocess for Manufacturing Human Pluripotent Stem Cell-Derived Endothelial Cells

— **Ou Wang**, Qian Du, Qiang Li, Haishuang Lin, Bin Duan, Yuguo Leo Lei

Paper 176n: Microfluidic Approaches to the Study of Chemotropism in Plant Cells

— Naoki Yanagisawa

Paper 176o: Hitting Undruggable Targets: Design of Double-Click Stabilized p_{s3}-like Peptides with Serum-Independent Efficacy

— **Lydia Atangcho**, Tejas Navaratna, Kirsten Deprey, Joshua Kritzer, Greg Thurber

Paper 176p: Islet-Mimetic Organoid Vascularization Utilizing Microvascular Fragments

— **Connor Wiegand**, Joseph E. Candiello, Prashant Kumta, Jay Hoying, Ipsita Banerjee

Paper 176q: Engineered Fn₃ Proteins Have Therapeutic Effect on Mesothelin-Expressing Cancer Cells — *Allison R. Sirois, Daniela A. Deny,*

Yanxuan Li, Yacine D. Fall, Sarah J. Moore

Paper 176r: Mitigating Antagonism Antagonism between Transcription and Proliferation Allows Near-Deterministic Cellular Reprogramming

- Kate E. Galloway

Paper 176s: Development of Synthetic Lethal Drug Combinations Targeting Metabolic Vulnerabilities in Glioblastoma Cells

— **James Joly**, Belinda Garana, Phil Phung, Sydney Parrish, Nicholas A. Graham

Paper 176t: The Metabolic Impact of Radiation Damage within the Tumor Microenvironment

— Kevin Corn, Marjan Rafat

Paper 176u: Raps: Rapid Annotation of Photosynthetic Systems

— Alexander Metcalf, Michelle Meagher, Anthony Nagygyor, Walter Prentice, Emily Bournia, Stuart Ramsey, Nanette R. Boyle

Paper 176v: Miren: An Optimization Tool for Transcriptomic Data-Driven Discovery of Global Regulatory Phenomena during Heat Stress in Rice Seed

– Mohammad Mazharul Islam, Jaspreet Sandhu, Harkamal Walia, Rajib

Paper 176w: Comparison of Community Detection Algorithms in Biological Networks from a Topological and **Functional Perspective**

- Sara Rahiminejad, Mano R. Maurya, Shankar Subramaniam

Paper 176x: Polymeric Particle Based **Endotoxin Removal from Protein** Solutions

- **Sidharth Razdan**. Sutapa Barua

Paper 176y: Quantitative Analysis of the Plasma Membrane Outer Leaflet in Red **Blood Cells**

Amid Vahedi, Amir M. Farnoud

Paper 176z: A Metagenomic Search Successfully Identifies Natural Amine Dehydrogenases with High Accuracy - Adam A. Caparco, Eric Pelletier, Jean-Louis Petit, Veronique de Berardinis, Anne Zaparucha, Julie A. Champion, Andreas S. Bommarius, Carine Vergne-Vaxelaire

Paper 176aa: Modulating Lipid Droplet Breakdown in Mammalian Cells through a Split Mediated Interaction

- Mitch Raith, Paul Dalhaimer

Paper 176ab: LambdaFabSelect High Throughput Method for Clone Selection in Duetmab Molecules

- Dhanesh Gadre

Paper 176ac: Integrative Cellular and Nuclear Dynamics in Single-Cell Imaging Analysis

— Tian Lan

Paper 176ad: Cell Cycle Progression Drives the Transitions between Epithelial and Mesenchymal Phenotypes

— **Tian Lan**, Yiider Tseng, Weisheng Chen

Paper 176af: Understanding the Metabolism of Cancer Persisters

- **Prashant Karki**, Mehmet Orman

Paper 176ag: Phospholipid Remodeling Via Exogenous Polyunsaturated Fatty Acid Uptake Modulates Stress Resistance in Vibrio Cholerae

- William Strike, Konner Glass, Bradley Harris, David Giles

Paper 176ah: Modeling the Adhesive Behavior of Platelets during Coagulation - Megan Cala, Robert S. Parker, Joseph J. McCarthy

Paper 176ai: Targeting DNA Repair Mechanisms in Bacterial Persisters - Sayed Golam Mohiuddin, Thao Vy Nguyen, Mehmet Orman

Paper 176aj: Targeted Pulmonary Drug Delivery in COPD Patients

- Ahmadreza Haahneaahdar, Rahul Bharadwaj, Yu Feng, Saurabh Sarkar

Paper 176ak: Influence of Fluid Properties for Needle-Free Jet Injection of Nucleic Acid Vaccines

— Jeremy Marston

Paper 176am: Title: Modeling and Simulation of Magnetophoresis of Nanoparticles - Physical Insights into Magnetic Targeting Applications

- Ayankola Ayansiji, Anish V. Dighe, Andreas Linninger, Meenesh R. Singh

Paper 176an: Ternary Amorphous Solid Dispersions – an Investigation Onto the Effects of the Addition of Mesoporous Silica on the Physicochemical Properties and Release Profile

- Samuel Solomon, Ahmad B. Albadarin

Paper 176ao: Roles of Regulatory Proteins in Controlling Endocytosis of siRNA-Containing Complexes

- R. Chauncey Splichal, S. Patrick Walton, Christina Chan

Paper 176ap: Effect of Delivery Vehicle Surface Charge on the Intracellular Trafficking of Sirnas

- Daniel Vocelle, Christina Chan, S. Patrick Walton

Paper 176aq: Porous and Degradable HA Particles As Sustainable Multiple **Drug Releasing Capabilities**

- Selin S. Sagbas, Saliha B. Kurt, Ramesh S Ayyala, Nurettin Sahiner

Paper 176ar: Loading and Dynamics of Doxorubicin on Pegylated Graphene Oxide Nanocarriers By Molecular **Dynamics Simulation**

- Mina Mahdavi, Ali Fattahi, Emad Tajkhorshid, Sasan Nouranian

Paper 176as: Vitamin-E Integrated Contact Lenses for Glaucoma Treatment — **Poorvajan Sekar**, Anuj Chauhan

Paper 176at: Hydrogels for Biomedical Applications: Characterization of Structure and Performance Via NMR Relaxometry

- **Alan Allgeier**, Brandon Kinn

Paper 176au: Investigating the Impact of a Nanocarrier Physiochemical Properties on Penetration into Ocular Surface Barriers

— Marjan Azadi, Allan E. David

Paper 176av: Understanding Nanoparticle Distribution within the Peritoneal Cavity for the Treatment of Ovarian Cancer Metastasis

— Derek Hargrove, Syed Ahsan, Bodhisattwa Chaudhuri, Xiuling Lu, Andrew Salner

Paper 176aw: Rifampicin-Cyclodextrin Inclusion Complexes Formulated for Pulmonary Drug Delivery

- **Matthew Freeman**, Stephanie Barneman, Samantha A. Meenach, Jie

Paper 176ax: Carbon Monoxide Concentration in Mainstream E-Cigarette Effluent Measured with Diode Laser Spectroscopy

- Dabrina Dutcher, Karen Castle

(177) Poster Session: Food and **Bioprocess Engineering**

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Nuttha Thongchul, Chair Yan Li, Co-Chair Hongxin Fu, Co-Chair

Sponsored by: Food

Paper 177a: Preparation of Functionalized Tilapia Fish Skin Collagen Peptide By Spsn-Immobilized Protease and Their Anti-Oxidation Component Analysis – Kaijun Xiao

Paper 177b: Cleaning of Substrates Using High Pressure Carbon Dioxide Mixtures: Flow Field & Fluid Composition

Effects on Biofilm Removal - Leah W. Falade, Gifty Osei-Prempeh, Kenneth L. Roberts

Paper 177c: Cinnamon, Rosemary and Oregano Essential Oils Nanoemulsions Used As Antimicrobials in Celery Juice - Mónica Dávila-Rodríguez, Aurelio

López-Malo, Enrique Palou, Nelly Ramírez-Corona, María Teresa Jiménez-Munguía

Paper 177d: Transpiration Rates of Leafy Vegetables during Postharvest Storage: Gravimetric and Theoretical Approach

— Betina Louise Angioletti, Stefany Pergentino dos Santos, Tuany Gabriela Hoffmann, Sávio Leandro Bertoli, Carolina Krebs de Souza

Paper 177e: Correlation of Rheological Characterisation of Honey with Its **Antibacterial Activities**

-Vincent Anidiobu

Paper 177f: Engineering Properties and Drying Characteristics of Cocoyam - Chijioke E. Onu, Joseph T. Nwabanne, Philomena Igbokwe

Paper 177g: Isosteviol Preparation and Inclusion Complexation of It with Γ-Cyclodextrin

– Hui-da Wan

Paper 177h: Study of Specific Refrigerated Storage Conditions for Minimally Processed Foods: A Review — Tuany Gabriela Hoffmann, Betina Louise Angioletti, Sávio Leandro Bertoli, Carolina Krebs de Souza

Paper 177i: Grape Residue Anthocyanin Extraction Using Ultrasound

- Rafael A. Batista de Medeiros, Oscar da C. Ferreira Neto, Gabriel C. Bevilaqua, João H. Fernandes da Silva, Edvaldo Vieira da Silva Jr., Shirley C. Rupert Brandão, Patricia M. Azoubel

Paper 177j: Effect of Ultrasound in Bioactive Compounds of Acerola Juice - Eunice G. Fraga Neta, Zilmar M. Pimenta Barros, Carlos B. Oliveira de Carvalho, Rafael A. Batista de Medeiros. Shirley C. Rupert Brandão, Patricia M. Azoubel

Paper 177k: Design and Characterization of a UVC-Coiled Tube Reactor and Continuous Flow Microwave System for Pasteurization of Juices

— Diana Laura Gomez-Sanchez, **Nelly** Ramírez-Corona, Aurelio López-Malo,

Paper 177I: Folic Acid Stability in the Gummy Matrix: Key Factors — Haiyan Ge

Paper 177m: Unravelling the Mechanisms of Resistance of Escherichia coli, Salmonella, and Listeria biofilms to Cold Atmospheric Plasma, As Affected By Age and Surface Physico-Chemistry

- Hani El Kadri, Jorge Gutierrez-Merino. Philip Thomas. Gavin Sandison. Thomas Harle, Tom Wantock, Andrea Lucca Fabris, Eirini Velliou

Paper 177n: Modelling the Growth of Listeria in Novel Viscoelastic Biphasic Systems Rich in Fat with/without the Presence of Nisin or Nisin-Producing Lactococcus Lactis

- Hani El Kadri, Jorge Gutierrez-Merino, Eirini Velliou

Paper 177o: Butanol Production from Hydrolysate of Jerusalem Artichoke Tubers By Clostridium Acetobutylicum - Lijie Chen, Youduo Wu

Paper 177p: Enhanced Hydrogen Production from Non-Sterilized Lignocellulose Hydrolysates By Nfnab-Deleted Thermoanaerobacterium Aotearoense SCUT₂₇
— **Jufang Wang**, Hongxin Fu, Yang Li

Paper 177q: Engineering of Clostridium Carboxidivorans for Enhanced Ethanol and Butanol Production from Syngas and Glucose

- Chi Cheng, Weiming Li, Meng Lin, Chuang Xue, Shang-Tian Yang

Paper 177r: N-Butanol Production in Clostridium Tyrobutyricum Triggered By Overexpression of Hydrogenase - **Weiming Li**, Chi Cheng, Guangli

Cao, Nangi Ren, Shang-Tian Yang

Paper 177s: Engineering Yarrowia Lipolytica for Efficient Production of Plant-Derived Very Long-Chain Monounsaturated Fatty Acid-Nervonic Acid — Tianqiong Shi, Xiao-Jun Ji

Paper 177t: Bioprocess Optimization Production By Saccharoplyspora Erythraea from Bench to Semi-Industrial Scale - Roslinda Abd Malek, Mohamed Ali Mohamud, Solleh Ramli, Siti Zulaiha Hanapi, Dalia Sukmawati, Hesham EL **Enshasy**

Paper 177u: Volumetric Oxygen Transfer Coefficient As a Parameter for Scale-up Probiotic Bacteria Production (Lactobacillus fermentum K₇₃) - **Arjana Serrano Delgado**, María Ximena Quintanilla Carvajal

Paper 177y: Statistics Guided Systematic Engineering for High-Yield Production of Terpenoids in Auxotrophic Escherichia coli

- Sudha Shukal, Xixian Chen. Conggiang Zhang

Paper 177v: High Magnetic Energy Gradient Quadrupole Magnet to Fractionate Oxirase-Deoxygenated Low Iron Label-Less RBCs from Aged Blood Donations

- Mitchell Weigand, Jeffrey Chalmers

Paper 177w: Pd@Pt Nanoparticle-Amplified Immunoassay for Rapid Detection of Harmful Herbicides

— **Eunice Kwon**, Xiaofan Ruan, Limin Wang, Yuehe Lin, Dan Du, Bernard J. Van Wie

Paper 177x: Dorsoventral Polarity Regulates the Modes and Mechanisms of Cell Migration in Confinement

— Panagiotis Mistriotis, Emily Wisniewski, Kaustav Bera, Robert Law, Soontorn Tuntithavornwat, Alexandros Afthinos, Runchen Zhao, Petr Kalab, Konstantinos Konstantopoulos

(178) Poster Session: Food Innovation and Engineering Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

David E. Block, Chair

Sponsored by: Food Innovation and Engineering

Paper 178a: Additive Manufacturing of Food: Formulation and Printability Criteria — Azarmidokht Gholamipour-Shirazi, Tom Mills

Paper 178b: The Possible Application of a Single Passive Acoustic Emission Sensor to Identify Different Complex Fluids in a Fully Flooded Pipe

— Daniel Ingo Hefft, **Federico Alberini**

Paper 178c: Event-Based Optimisation for Harvesting Scheduling Under Precision Agriculture

— **Qingyuan Kong**, Kamal Kuriyan, Nilay Shah**, Miao Guo**

Paper 178d: Antimicrobial Mesh Materials Applied to Milk and Brine — Mainara Costa-Teixeira, Shelby Brooks, M. Preston Richier, Ryan M. Summers, Stephen M. Ritchie

Paper 178e: Investigation of Pipe Cleaning Process Using Planar Laser Induced Fluorescence

— Min Zhang, **Federico Alberini**, Kylee R. Goode, Katharina Roettger, **Peter J. Frver**

Paper 178f: Steam Stripping of Aroma from Coffee: Multi Scale Modelling of Extraction Behaviour

— David Beverly, **Peter J. Fryer**, Serafim Bakalis, Estefania Lopez-Quiroga, Robert Farr

Paper 178g: Model Reduction of Phase-Field Models Describing Crystallisation Phenomena

— **Estefania Lopez-Quiroga**, Peter J. Fryer Paper 178h: Oleogels As Future *Trans* fat Alternative: A Mathematical Model for an Unsolved Conundrum in Gelation during Scale up Process

— **Sai Sateesh Sagiri**, Malick Samateh, Shihao Pan, Charles Maldarelli, George John

(179) Poster Session: General Poster Session in Sensors

Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

Jeffrey M. Halpern, Chair C. Wyatt Shields IV, Co-Chair

Sponsored by: Sensors

■ MICRO/NANO WIRES

Paper 179a: Oriented Freeze-Casting Fabrication of Resilient Copper Nanowire-Based Aerogel As Robust Piezoresistive Sensor

— **Jiankun Huang**, Baoqiang Liang, Zifeng Yan

Paper 179b: Synthesis of Core-Shell Palladium Nanowires@ZIF-8 for Hydrogen Sensors

— **Abhishek Kumar**, Yi Chen, Mark T. Swihart

Paper 179c: Charge-Transfer Salt Nanowire Electrocrystallization for Ammonia Detection

— **Xuecheng Yu**, Mohamed Kilani, Guangzhao Mao

Paper 179d: Synthesis and Characterization of Charge Transfer Complex Micro/Nanowire Junctions and Their Application in Gas Sensing

— **Mohamed Kilani**, Xuecheng Yu, Guangzhao Mao

BIOSENSORS

Paper 179e: Biomimetic Properties of Modified Graphene Oxide and Graphitic Carbon Nitride Nanomaterials for Biosensing Applications

— Muhammad Nasir

Paper 179f: Biosensors Using Metamaterial-Inspired Ring Resonators

— **Sangeeta Kale**, Sweta Rath, Vivek Kale, Chetan Chavan, Shankar Gaware, Vaishali Rawat

Paper 179g: Fabrication of Laser Printed Microfluidic Paper-Based Analytical Devices for Point-of-Care Applications

— Rajesh Ghosh, Saranya Gopalakrishnan, Rangasamy Savitha, Thiruvengadam Renganathan, Subramanium Pushpavanam

Paper 179h: Modeling Fermi Levels in Metal Functionalized TiO₂ Sensors for Applications in Volatile Organic Biomarker Detection Associated with Pneumonia

— **Lani McKinnon**, Yalda Saffary, Krista Carlson, Swomitra Mohanty

GAS PHASE SENSORS

Paper 179i: Factors Affecting CO₂
Accumulation in the Motor Vehicle Cabin
— Yue Deng, Mark Sprowls, Doina
Kulick, Nongjian Tao, Hugo Destaillats,
Erica Forzani

Paper 179j: Curating Metal-Organic Frameworks to Compose Robust Gas Sensor Arrays

- Arni Sturluson, Cory Simon

NMR OR PLASMON

Paper 179k: Probe Design for NMR of Chemical Reactions at High Temperature and Pressure

— **Hilary T. Fabich**, Partha Nandi, Hans Thomann, Mark S. Conradi

Paper 179I: Sensing and Detection of Arsenic By Localized Surface Plasmon Resonance of Gold-Vitamin B₁₂ Complex and a Device Thereof

— Prithwish Biswas, **Rajdip Bandyopadhyaya**

(180) Poster Session: Interfacial Phenomena (Area 1C)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom M Raymond Tu, Chair Marina Tsianou, Co-Chair Mark Kastantin, Co-Chair

Sponsored by: Interfacial Phenomena

Paper 180a: Prediction of Transition Regime Properties in a Bubble Column Under Various Gas-Liquid Systems — Hanjin Im, Jeil Park, Jae W. Lee

Paper 180b: Effect of Surfactants and Nanoparticles on Emulsions Stability — *Abeer Khedr, Alberto Striolo*

Paper 180c: Clathrate Hydrate-Water Interfacial Dynamic Behaviors with the Precipitation of Metal Naphthenate

— Wonhyeong Lee, Juwon Min, Yun-Ho Ahn, Seungjun Baek, Carolyn A. Koh, Jae W. Lee

Paper 180d: Potassium Copper Hexacyanoferrate-Embedded Doubly-Crosslinked Magnetic Hydrogel for Effective Cs* Removal and Facile Recovery

— **Yun Kon Kim**, Kyeonghui Bae, Yonghwan Kim, David Harbottle, Jae W. Lee

Paper 180e: Friction As a Means of Detecting Biomolecules with Ultrahigh Sensitivity and Specificity

— **Bakdaulet Isakhov**, W. T. Godbey, Noshir S. Pesika

Paper 180f: Effects of Inhibited Oligonucleotide Transport on Interfacial Hybridization and Molecular Searching

— Jeremiah Traeger

Paper 180g: Understanding the Cooperative Adsorption of Globular Proteins

— **Jin Gyun Lee**, Yao Wu, Kelly Lannigan, Luke L. Larive, William A. Shelton Jr., Bhuvnesh Bharti

Paper 180h: Substrate Controlled Synthesis of Organic Nanowires for Sensor Applications

— **Xuecheng Yu**, Mohamed Kilani, Guangzhao Mao Paper 180i: Nanorheological Behaviors and Flow Dynamics of Isotropic/ Anisotropic Geocolloids in Aqueous Medium

— **Yuanzhong Zhang**, Younjin Min, Stephen Merriman

Paper 180j: Conformational Orientation of Monoclonal Antibody at the Air-Water Interface

— Ankit Kanthe, Mary Krause, Songyan Zheng, Andrew Ilott, Jinjiang Li, Wei Bu, Mrinal Bera, Binhua Lin, Charles Maldarelli, Raymond Tu

Paper 180k: Phase Transfer Catalyst
-Functionalized Nanosheets for
Emulsion Formation and Stabilization
— Nishat Anjum, Ya-Wen Chang

Paper 1801: Investigation of Lateral Drop Motion By Centrifugal Adhesion Balance (CAB)

— Akash Jena

Paper 180m: Determination of Dynamic Interfacial Tension in a Pulsed Disc and Doughnut Column

— **Bo Wang**, Shaowei Li, Shan Jing

Paper 180n: Two-Phase Faraday Resonance with Patterned Substrates-Theory and Experiments

— **B. Dinesh**, Nevin Brosius, Farzam Zoueshtiagh, Ranga Narayanan

Paper 180p: Superhydrophobic Nanorod Arrays for Enhancing Water Condensation Heat Transfer

— **Jiayu Song**, King Lun Yeung

Paper 180q: Lipid Headgroup Regulates the Disruption of Lipid Membranes By Silica Nanoparticles

— **Saeed Nazemidashtarjandi**, Amir M. Farnoud

Paper 180r: Effect of Charge and Fluctuation of Vesicle Membranes on the Oligomerization of Aniline
— Saki Fukuma, Toshinori
Shimanouchi, Yukitaka Kimura

Paper 180s: Endothelial Membrane Biomechanics Under Dyslipidemic Conditions

— Manuela A.A. Ayee, Irena Levitan

Paper 180t: Understanding of Liquid-Liquid Mass Transfer at High pH and Salt Concentrations

- Jeil Park, Shinbeom Lee, Jae W. Lee

(181) Poster Session: Materials Engineering & Sciences (08A -Polymers)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S Julianne L. Holloway, Chair

Amy M. Peterson, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

THIN FILMS, SURFACES, AND **COATINGS**

Paper 181a: Fabrication of Nanostructures Via Directed Self-Assembly of Block Copolymers

- **Dong-hyun Kim**, Jinju Bae, Seo Hyun Park, Jongwan Ko, MyungHwan Byun, Man Sig Lee

Paper 181b: Confinement Effects on Dye Translational Diffusivity in Polystyrene Thin Films Depend on Polymer Molecular Weight: Connection to Fragility-Confinement Effects

- Tong Wei, Tian Lan**, John M.** Torkelson

Paper 181c: Glass Transition Temperature of a Polymer Thin Film: Simulation Methodology and Statistical Variation

David McKechnie, Jordan Cree, Karen Johnston

Paper 181e: Monolayer Two-Dimensional Polymers for Wafer-Scale Heterostructures

Yu Zhong, Baorui Cheng, Chibeom Park, Ariana Ray, Sarah Brown, Fauzia Mujid, Jae-Ung Lee, Hua Zhou, Joonki Suh, Steven J. Sibener, David A. Muller, Jiwoong Park

Paper 181f: Block Copolymer Directed Self-Assembly Defect Modes Induced By Localized Errors in Chemoepitaxial Guiding Underlayers: A Molecular Simulation Study

- Jakin B. Delony, Peter J. Ludovice, Clifford I Henderson

Paper 181g: High Pressure Impregnation of Alkyl Ketene Dimers (AKD) in Cellulose Substrates, Creating Novel Sticky Hydrophobic Surfaces

- Brenda Hutton-Prager, Kolawole Adenekan

Paper 181h: Effects of HPHT Conditions on the Rate of Degradation of High Performance Epoxy Coatings

– Narayanan Rajagopalan, Claus Erik Weinell, Kim Dam-Johansen, Søren Kiil

Paper 181i: Tailoring Surface Wettability of 3-D Printed Minimal Surfaces Using iCVD for Implementation As Packing in Gas-Liquid Absorption Columns

– Aravind Suresh, James P. Abulencia, Robert C. Ryan, Daniel D. Burkey, Adam Pangilinan

Paper 181j: Optical and Electrical

ENERGY

Properties of Solution-Mixed and Sequentially Processed Poly(3alkylthiophene):F,TCNQ Films - Zaira I. Bedolla-Valdez, Alice Fergerson, Alejandra N. Ayala-Oviedo, Alexia A. Portillo, Zigra Raza, Jiawei Guo, Adam J. Moulé

Paper 181k: High Electron Affinity Molecular Dopants for Solution **Processing of Organic Semiconductors** - Goktug Gonel, Jan Saska, Rachel Talbot, Alice Fergerson, Margaret Riley,

Zaira I. Bedolla-Valdez, Sean D. Aronow, Fengyu Zhang, Nikolay E. Shevchenko, Antoine Kahn, Alexander S. Dudnik, Mark Mascal, Adam J. Moulé

Paper 1811: Fmoc Assisted Gelation of P₃HT

– Madhubhashini Lakdusinghe, Rangana Wijayapala**, Santanu Kundu**

Paper 181m: Tuning the PEDOT Lattice Parameter By Engineering Dopant Level for Efficient and Stable Perovskite Solar Cell Device

– Meysam Heydari **Gharahcheshmeh**

Paper 181n: Synthesis of Supercapacitor Electrodes Based on Polyaniline Microfibers Using a Novel **Electrospinning Architecture**

— **Somdatta Bhattacharya**, Aaron Tice, Caitlyn Chapman, Indroneil Roy, Vidhya Chakrapani, Joel L. Plawsky, Robert J. Linhardt

Paper 181o: Stabilizing Electroconvective Flow in Viscoelastic Polymer Electrolytes

- Duhan Zhang, Lynden A. Archer

Paper 181p: Charge Transport in Nonaqueous Polyelectrolyte Solutions for Li-Ion Batteries: Ion-Ion Correlations and the True Transference Number from Molecular Dynamics Simulations

- Kara D. Fong, Julian Self, Kyle M. Diederichsen, Brandon M. Wood, Bryan D. McCloskey, Kristin Persson

Paper 181g: Electrolyte Chemistries with Responsive Polymers for Thermal Safety in Li-Ion Batteries

- Mark E. Roberts

Paper 181r: Magnesium Ion Conduction in Poly(ionic liquids) with Organic Cations

- Bumiun Park, Jennifer Schaefer

Paper 181s: Structure-Property Relationships in Dynamic Polymer Networks for Electrochemical Applications

Snehashis Choudhury, Yi Cui, Zhenan Bao

Paper 181t: Novel Polymer Nanocomposite Anion-Exchange Membranes Based on Ni₂+-Modified g-Carbon Nitride

Carla Zambrana-Cruz, Geovanna Santiago, Omar Móvil-Cabrera

WATER

Paper 181u: Porous Thin Films Via Physicochemical-Selective Initiated Chemical Vapor Deposition (iCVD)

- Mahdi Mohammadi Ghaleni, Mona Bavarian, Siamak Nejati

Paper 181v: Removal of Hg,+ from Polluted Water Using Molecularly Ion-Imprinted Silica Particles (MIIP) As Fibrous Composite with Polysulfone

- Rosemarie Ann I. Cuevas, Grace M. Nisola, Khino J. Parohinog, Erwin C. Escobar, Wook-Jin Chung, Lawrence A. Limjuco

Paper 181w: Development of Novel Crosslinked Polymers with Intramolecular Pi-Pi Interactions - Rishabh Shah. Thomas Dziubla, J. Zach Hilt

Paper 181x: Compatible Zwitterion-**PVDF Membrane Designs**

– Amira Abdelrasoul

Paper 181y: Multicomponent Transport in Hydrated Dense Polymer Membranes: Impact of Varied Fractional Free Volume - Breanna M. Dobyns, Jung Min Kim, Bryan S. Beckingham

Paper 181z: A Robust Cotton Textile Based Material for High Flux Oil-Water Separation

- Hongshuang Guo, Lei Zhang, Jing Yang

BIOMEDICAL

Paper 181aa: Investigation of PVA Microneedle for Protein Delivery

— Raquel de Castro, Hazim Aljewari, Audie Thompson

Paper 181ab: Rapid and Complete Implantation of Layer-By-Layer Microneedle Drug Films for Enhanced Transdermal Vaccination

- Yanpu He, Celestine Hong, Jiahe Li, MayLin Howard, Yingzhong Li, Michelle Turvey, Divakara Uppu, John Martin, Ketian Zhang, Darrell Irvine, Paula T. Hammond

Paper 181ac: Aqueous Media Resistant PVA/HPMC Nanofibers By Electrospinning Technique for Drug **Delivery System**

— Mar Calzado Delgado, M.O. Guerrero-Pérez, King Lun Yeung

Paper 181ad: Zwitterionic Polyurethanes with Tunable Surface and Bulk Properties

- Huifeng Wang, Gang Cheng

Paper 181ae: Tough Hydrogel Network Based on Calcium-Crosslinked Sulfur Salt — **Jesse Vongnaraj**, Ameya Narkar, Kollhe Ahn

Paper 181af: Polymer Coated Nanoparticles for Photothermal Therapy and Prognosis of Breast Cancer — Muhammad Raisul Abedin, Sutapa

STRUCTURE AND PROPERTIES

Paper 181ah: Polymer Based Cost-Effective Triboelectric Nanogenerator — Aminur Rashid Chowdhury, Diana Lopez, Abu Musa Abdullah, M. Jasim Uddin

Paper 181ai: Study on the Novel Porous PDMS-Based Dielectric Elastomer Actuators and Their Application in Robotics

— **Jiahui Xu**, Zhen Yao, Kun Cao

Paper 181aj: Uniaxial Compression of PVDF: A New Approach to Form Isotropic β Phase Thick Sheets - **Shubham Mireja**, Devang V.

Paper 181ak: Ultra-Stretchable P(AAMP-SA)/PANI/PA Conductive Polymer Complex with Excellent Linearity and Repeatable Autonomous Self-Healing Ability — Yang Lu, Jesse Horne, Lauren Mc-Loughlin, Rachel Ploeger, Ju-Won Jeon, Evan K. Wujcik

Paper 181al: Characterization and Evaluation of PMMA Interfacial Cohesion **Under Various Bonding Conditions** Pei-Kang Sun, R. S. Besser

Paper 181am: Prediction of Swelling and Linear Viscoelasticity of Starch Suspensions

— Gnana Prasuna Desam, Jinsha Li, Nadar Laal Dehghani, Vivek Narsimhan, Ganesan Narsimhan

Paper 181an: Conformational Rearrangement of Knots in Tensioned **Polymer Chains**

- Beatrice W. Soh, Alexander Klotz, Patrick S. Doyle

Paper 181ao: Analysis of Brownian Dynamics and Molecular Dynamics Data of Unentangled Polymer Melts Using Proper Orthogonal Decomposition - Chi Pui Jeremy Wong, Phillip Choi

Paper 181ap: Coarse Grained Simulations for Observing Macromolecular Behavior Under Stress - Louise Kuehster, Tuan V. Vu, Dimitrios V. Papavassiliou

Paper 181aq: Performance of Phthalates and Alternative Plasticizers in PVC Via Molecular Simulation: Materials **Properties and Migration Tendency** - Dongyang Li, Kushal Panchal,

Paper 181ar: Accelerated Design of Molecular Additives for Polymer Crystallization

Roozbeh Mafi, Li Xi

- Corinne L. Carpenter, Gregory C. Rutledge, Richard D. Braatz

Paper 181as: Graphene Nanoscrolls Induced Crystallization of Polylactic Acid - Dilip Depan, Oluwakemi Ajala, Caroline Werther, Peyman Nikaeen

■ ADDITIVE MANUFACTURING

Paper 181at: High-Performance in-Situ Sequential Interpenetrating Network of Bismaleimide and Cyanate Ester for Vat Photopolymerization

- Anh Huynh, Nicolas J. Alvarez, Giuseppe Palmese

Paper 181au: Microcapsule-Based Self-Healing for 3D Printing - Vinita Shinde, Bryan S.

Beckingham, Asha-Dee Celestine

Paper 181av: Isosorbide-Based Low Viscosity Resins for Additive Manufacturing Applications

- Xi Chu, Heather Berensmann, John La Scala, Giuseppe Palmese

COMPOSITES

Paper 181aw: Structure and Dynamics in Matrix Free Polymer Grafted Nanoparticle Based Systems

- Mayank Jhalaria, Sanat K. Kumar

Paper 181ax: Effect of Thermal History on Particle Structure and Dynamics in Polymer Nanocomposites

- Andrew Jimenez

Paper 181ay: Effects of High Filler Content on the Thermal, Mechanical and Rheological Properties of Hnt/LLDPE Nanocomposite

— **Bahareh Baheri**, Sunggyu Lee

Paper 181az: Modeling of Diffusion in **Epoxy Resin Composites**

- Patrick Krenn, Patrick Zimmermann, Michael Fischlschweiger, Tim Zeiner

Paper 181ba: Analysis and Review of Micro and Nano-Structured Polymeric Materials

— Nikhil Prakash

Paper 181bb: Multi-Scale Modeling of Fiber-Matrix Interphase

— **Salman Zarrini**, Cameron F. Abrams

■ REACTION ENGINEERING

Paper 181bc: ABC Polymeric Ionic Liquid **Triblock Terpolymers**

- Patrick Lathrop, Yossef A. Elabd

Paper 181bd: Synthesizing Novel Degradable Polymers with Tunable **Mechanical Properties**

— Whytneigh R. Duffie, Eswar Arunkumar Kalaga, Timothy M. Brenza, Travis W. Walker

Paper 181be: Bio-Based Thermosets Prepared Using Aza-Michael Addition of Furan and Isosorbide Building Blocks — **Xi Chu**, Anthony Clay, John La Scala, Giuseppe Palmese

Paper 181bf: Development of Covalent and Non-Covalent Crosslinked Temperature Responsive Polymeric Gels — **Rishabh Shah**, Tyler Runge, Thomas Ostertag, Shuo Tang, Thomas Dziubla, J. Zach Hilt

Paper 181bg: Performance Evaluation of Synthesized Gemini Cationic Surfactants Having Different Hydrophobic Tail and Spacer Length for Enhanced Oil Recovery

- S. M. Shakil Hussain, Muhammad Shahzad Kamal

Paper 181bh: The Epoxidation of Polybutadiene By Reaction-Controlled Phase-Transfer Catalyst

Li Xu, Liqian Zhu, Zhisong Li, Suyun Jie, Bo-Geng Li

Paper 181bi: Controlled Synthesis of Polyolefin Copolymers with Rapid Curability for Photovoltaic Cell Encapsulation

- Liqiong Luo, Kailun Zhang, Pingwei Liu, Bo-Geng Li, Wen-Jun Wang, Guanada Zhou

Paper 181bi: Molecular Architecture Vs Reaction Conditions: Comprehensive Modeling of Arget-ATRP of Styrene-Acrylonitrile Copolymerization

- Cecilia Fortunatti, Adriana Brandolin, Claudia Sarmoria, Mariano Asteasuain

Paper 181bt: Experimental Validation of **Deconvolution Theory**

- Raunil Rai

Paper 181bk: Mathematical Modeling of Dispersion Copolymerization of Styrene and Maleic Anhydride: Nucleation and Particle Growth

- Maria Giuliana Fontanelli Torraga, Reinaldo Giudici

Paper 181bl: A More Detail Study on Tgic, Simultaneous Effect of Molecular Weight, Comonemer Content and Comonomer Type

— Amirreza Badri, Saeid Mehdiabadi, João Sogres

Paper 181bm: Theoretical and Experimental Study of the Phase Inversion Point during the High-Impact Polystyrene (HIPS) Production Process – **Juan M. Maffi**, Gregorio R. Meira, Diana A. Estenoz

Paper 181bn: Simulation and Control of a Batch Suspension Polymerization Reactor

- **Abdollah Koolivand**, Hamzeh Farahzadi, Mohammad Shahrokhi

■ RHEOLOGY AND PROCESSING

Paper 181bo: Extensional Rheology of Aqueous Polymer Solutions in Filament Thinning and Microfluidic Contraction

— Athena E. Metaxas, Benjamin Micklavzina, Cari S. Dutcher

Paper 181bp: Extensional Flow of Associating Polymers: From Processing to Performance

Zachary R. Hinton, Aamir Shabbir, Nicolas J. Alvarez

Paper 181bq: Mathematical Modeling of Blown Film Extrusion Using the Discrete Slip-Link Rheological Model

- Matthew R. Dobbins, J. Carl Pirkle Jr., Marat Andreev, Gregory C. Rutledge, Richard D. Braatz

Paper 181br: Modification of Recycle-PET and Its Compression Molding Process Foamed By Supercritical CO.

- Yichong Chen, Tao Liu, Ling Zhao

Paper 181bs: Effect of the Long Chain Branched Structure of Modified PET on Its Extrusion Foaming Behaviors Under Supercritical CO.

— **Shun Yao**, Tao Liu, Ling Zhao

(182) Poster Session: Materials Engineering & Sciences (08B -**Biomaterials**)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Julianne L. Holloway, Chair Amy M. Peterson, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

■ BIOLOGICAL MATERIALS

Paper 182a: Vibration at Structural Resonance Frequency of Hydrophilic Substrates Enhances Biofilm Removal

— William Ballance, Inkyu Oh, Yang Lai, Mohamed Elhebeary, Taher Saif, Yuhang Hu, Hyunjoon Kong

Paper 182b: Evaluation of Nano-Metal Organic Frameworks Safety through Transpiration and Translocation in Celery (Apium graveolens)

- Sheena Anne H. Garcia, King Lun Yeung

Paper 182c: Investigation of Mechanical Properties of Femur and Tibia Articulations of Insect Joints

- **Michael Bae**, Shuhao Liu, Jun Kyun Oh. Mustafa Akbulut

Paper 182d: Elastocapillarity Pumps: Water Transport in Feathers

- Symone Alexander, M. Saad Bhamla

Paper 182e: Degradation of Taste and Odor Compounds with Cactus Mucilage **Extraction Enhanced Photo-Catalysis** Under Solar Light

— Tunan Peng, Alcantar Norma

DEVICES

Paper 182f: Characterization and Application of Aluminum Nitride-Based Flexible Surface Acoustic Wave Devices on Thermoplastic Polyethylene Naphthalate

- Leonardo Lamanna, Francesco Rizzi, Pradipta Das, Shuangming Li, Venkat R. Bhethanabotla, Massimo De Vittorio

Paper 182g: Biostable Conductive Nanocomposite for Implantable Subdermal Antenna

- Frank Curry Jr.

Paper 182h: Core-Shell Gallium/Polymer Microstructure for Thermal Responsive Implantable Electrode

Taehwan Lim, Huanan Zhang

HYDROGELS

Paper 182i: Structure-Function Relationships in Peptoid Cross-Linked Hydrogels

- Logan Morton, Mariah J. Austin, Adrianne M. Rosales

Paper 182j: Hydrogel Crosslinking By Minimally Invasive Surgical Modalities - Tasmia Tasnim, Huanan Zhang

Paper 182k: A Dynamic Hydrogel Platform for Cardiac Tissue Model - Andrew House, Murat Guvendiren Paper 1821: Supramolecular Hydrogels: Complex Rheological Behavior of Polymer-Nanoparticle Hydrogels and Its Impact on Drug Release Kinetics — Hector Lopez Hernandez, Eric A. Appel

NATURAL POLYMERS

Paper 182m: Understanding the Impact of Non-Natural Amino Acid Incorporation on the Assembly of Multifunctional Collagen Mimetic Peptides: Simulations and Experiments

- Phillip Taylor, Amber Hilderbrand, Arthi Jayaraman, April M. Kloxin

Paper 182n: Effective Immobilization of Potassium Copper Hexacyanoferrate Via Amino-Functionalization of Magnetic Chitosan Adsorbent for Selective Cs+ Separation

— **Hyelin Roh**, Yonghwan Kim, Yun Kon Kim, David Harbottle, Jae W. Lee

Paper 1820: Solution Phase Separation Using Deep Eutectic Solvents for the Fabrication of Chitosan-Based Porous Materials

- Luis Humberto Delgado-Rangel, Janett Betzabe Gonzalez-Campos, Josué Mota-Morales, Yliana Lopez-Castro, Judit Aviña-Verduzco

■ NEW METHODS

Paper 182p: D-7-ACA Dissolution in a Micromixer with a Circulator - Xie Yu, Yujun Wang

Paper 182q: Patterning Matrix Droplets for Quantitative Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging

- Sanghwan Park, Chang Young Lee

Paper 182s: Frozen Films: Porous Thin Films for in Vitro Culture — Kailei Xu, Dana Rowley**, Stephen**

Florczyk

■ THERAPEUTIC DELIVERY

Paper 182t: Quantitation of Zwitterionlike Succinylated Polyethylenimine/DNA Polyplex Intracellular Trafficking Kinetics - Levi Lampe, Logan Warriner, Daniel

Paper 182u: Characterization of Microfluidic Calcium Phosphate-Mediated DNA Delivery - Levi Lampe, Daniel W. Pack

Paper 182v: Thermoresponsive Protein Hydrogels for Sustained Delivery of **Small Molecules**

- Michael Meleties, Lindsay K. Hill, Priya Katyal, Xuan Xie, Erika Delgado-Fukushima, Teeba Jihad, Che Fu Liu, Sean C. O'Neill, Raymond S. Tu, P. Douglas Renfrew, Richard Bonneau, Youssef Z. Wadahiri, Jin Kim Montclare

Paper 182x: Protein Corona Formation on Pegylated Particles for Drug Delivery - Mark Bannon, Aida Lopez-Ruiz. Miriam Marquez, Karen Reyes, Zahra Wallizadeh, Mohammad Savarmand, Kathleen McEnnis

Paper 182y: A Data Analytics Approach for Rational Design of Nanomedicines with Programmable Drug Release

— **Adam Mullis**, Scott Broderick, Andrea M. Binnebose, Nathan Peroutka-Bigus, Bryan H. Bellaire, Krishna Rajan, Balaji Narasimhan

Paper 182z: Controlling Morphology of Biodegradable Polymer Particles with Bioactive Small Molecules and Its Application in Modulating Adipose Tissue Function

- Christopher Isely, Michael Gower

Paper 182aa: The Effect of Dispersed-Phase Solvent and Extraction Volume on Rosiglitazone Encapsulation in PLG Particles

— **Christopher Isely**, Madeline Spetz, Michael Gower

Paper 182ab: Drug Delivery System for Platinum Nanoparticles

Platinum Nanoparticles
— *Aida Lopez-Ruiz*, *Kathleen McEnnis*

Paper 182ac: Development of Polymeric Thin Films for Local Delivery of siRNA

— **Jonathan Chou**, Adam G. Berger, Paula T. Hammond

Paper 182ad: Fabrication of Porous Polysaccharide Based Biomaterials with Active Therapeutic Delivery Capability Using Supercritical CO₂

— **Gregor Kravanja**, Željko Knez, Mateja Primozic, Maja Leitgeb

Paper: Soft Nanocapsules for Systemic Gene Delivery

— Hyungjun Kim, Yoon Yeo

■ TISSUE ENGINEERING

Paper 182ae: Combining Phosphorylated Chitosan-Xanthan Complexes and PCL to Obtain Bilayered Periosteum-like Scaffolds for Bone Regeneration

— **Renata F. Bombaldi de Souza**, Ângela Maria Moraes

Paper 182af: Development of Injectable Hydrogels for Cartilage Tissue Engineering

— Ângela Maria Moraes, Cecília Buzatto Westin, Camila Medeiros Fonseca, Mariana Harue Taniguchi Nagahara

Paper 182ah: The Incorporation of Bio-Inspired Polymeric Coatings for Enhanced Schwann Cell Proliferation and Stem Cell Differentiation

— **Jesse Roberts**, Luis Carlos Pinzon-Herrera, Joshua Corbitt, Shannon L. Servoss, Jorge Almodovar

Paper 182ai: Biocompatibility of Polyampholyte Polymers for Tissue Engineering Applications

— **Stephanie Haag**, Matthew T Bernards (183) Poster Session: Materials Engineering & Sciences (08D -Inorganic Materials)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Julianne L. Holloway, Chair Amy M. Peterson, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

CATALYSIS

Paper 183a: N Self-Doped Pollen-like Macroporous Carbon for Selective Hydrogenation of 1, 3-Butadiene

— Daohua Sun, Qingbiao Li

Paper 183b: Enhanced Hydrogen Evolution from the Heterostructure Photocatalysts

— Jung Hyeun Kim

Paper 558ab: Ru Atoms Immobilized on Porous Hexagonal Boron Nitride for CO₂ Methanation

— **Juan Jimenez**, Mengmeng Fan, Jingjie Wu, Donping Sun, Pulickel M. Ajayan, Jochen Lauterbach

COVALENT ORGANIC FRAMEWORKS

Paper 183d: In Situ Bottom-up Synthesis of Porphyrin-Based Covalent Organic Frameworks

— Elham Tavakoli, Shayan Kaviani, Mahdi Mohammadi Ghaleni**, Siamak Nejati**

Paper 183e: Investigating the 3-D Self-Assembly of Chemically Specific Building Blocks for Covalent Organic Frameworks

— **Tiara Ann Maula**, Srinivas Rangarajan, Jeetain **M**ittal

■ METAL ORGANIC FRAMEWORKS

Paper 183g: Microfluidic Approach Toward Continuous Synthesis of HKUST-1 Using 3D Printing Technology — Paria Coliaie, Meenesh R. Singh

Paper 183h: Modeling the Reactivity of Open Metal Sites in Metal Organic Frameworks for Olefin Paraffin Separation

— Lin Li, Mona H. Mohamed, Yahui Yang, Sen Zhang, Kushantha Withanage, Juan Peralta, Koblar Jackson, Götz Veser, Nathaniel L. Rosi, J. Karl Johnson

Paper 183i: Metal-Organic Frameworks for Photonics Functional Applications

— **Yuanjing Cui**, Guodong Qian

Paper 183k: Laser-Induced Synthesis of Metal Organic Frameworks (MOF): A Facile Approach for the Fabrication a Wide Range of Crystalline MOFs and Their Functional Composites

— **Erick L. Ribeiro**, Dibyendu Mukherjee, Bamin Khomami

Paper 183I: Computational Design of Metal–N-Heterocyclic Carbene Complexes Immobilised in a Metal–Organic Framework for CO₂ Hydrogenation — Kuiwei Yang, Jianwen Jiang

Paper 183m: Conversion of Hydroxy Double Salts for Scalable Synthesis of Metal-Organic Frameworks

— Yixin Chen, Yingwu Luo, Junjie Zhao

METALS

Paper 183n: High-Yield Production of Boron-Based Nanosheets from Magnesium Diboride By Dissolution and Recrystallization in Water

— **Harini Gunda**, Saroj Kumar Das, Kabeer Jasuja

Paper 183o: Modification of Metal Surfaces with Superhydrophobic Nanotextures for Enhanced Food Safety and Hygiene

— **Shuhao Liu**, Michael Bae, Jun Kyun Oh, Mustafa Akbulut

Paper 183r: Optimal Design of Novel Precursor Materials for Atomic Layer Deposition Using Computer Aided Molecular Design

— **Mina Shahmohammadi**, Rajib Mukherjee, Christos G. Takoudis, Urmila M. Diwekar

PARTICLES

Paper 183s: Evaluation of the Influence of Fine Particle Surface Modification with Thehansen Solubility Parameters

— **Nobuyuki Fujiwara**, Hideki Yamamoto Sr.

Paper 183t: The Role of Aminosilane Loading Density on the Formation of Gold- Coated Superparamagnatic Core/ Shells with Enhanced Dual Surface Heating to Combat Tumor

— Manal Almusaynid

Paper 183u: Preparation and Characterization of Hollow Flower-like Nickel Nanoparticles

— **Teng Zhang**, Tao Wang

Paper 183v: Tuning Uio-66 Particle Size, Defectiveness, and Fluorescence Via Modulation of Water and Ligand Equivalents

— **Zachary Stillman**, Jay Decker, Lucas Attia, Eric Bloch, Catherine A. Fromen

PURIFICATION

Paper 183w: Thin and Highly Selective Molecular Sieving Membranes for Cost Effective Hydrogen Purification

— **Marie Bermeo**, Safiya Khalil, Maryam Khaleel

Paper 183y: Preparation and Characterization of a Novel Electrospun Activated Carbon/Whey Protein/ Polycaprolactone Membrane for Heavy Metals Removal

— Laura Cristina Ramírez-Rodríguez, María Ximena Quintanilla Carvajal, Edisson Tello, Carlos A. Jiménez-Junca

ZEOLITES

Paper 183z: Elucidating the Factors Governing Organic-Free Interzeolite Transformation

— **Rishabh Jain**, Jeffrey D. Rimer

Paper 183aa: Dual Role of Surfactants As Structure-Directing Agents and Mesoporogens in the Preparation of Zeolites

— **Aseem Chawla**, Noemi Linares, Rui Li, Rishabh Jain, R. John Clark, James Sutjianto, Jeremy C. Palmer, Javier García-Martínez, Jeffrey D. Rimer

Paper 183ab: A Commercially-Viable One-Step Synthesis Method to Prepare MWW Zeolite Nanosheets

— **Yunwen Zhou**, Ming-Feng Hsieh, Bernd Kabius, Yanyu Mu, Robert Rioux, Jeffrey D. Rimer

Paper 183ac: The Synthesis of Zeolites with High Specific Surface Area and Their Application in VOCs Adsorption Removal

- Shuangchun Lv

Paper 183ad: Li and Mg Ion-Exchange of Zeolite NaX Coatings Crystallized on Metal to Obtain Materials with Enhanced Water Sorption Capacity

- Cigdem Atalay-Oral, Melkon Tatlier

CERAMICS

Paper 183ae: Effects of [Zn_{0.5}Si_{0.5}]3+ Substitution on Microwave Dielectric Properties of ZnAl₂-X(Zn_{0.5}Si_{0.5})xO₄ Ceramic

— Xuekai Lan, Jie Li, Jiapu Li, Wen Lei

Paper 183af: Lattice Structure Analysis and Optimized Microwave Dielectric Properties of MgAl(2-2x)(Mg_{0.5}Ti_{0.5})₂xO₄ Compounds with Spinel Structure — Jie Li, Xuekai Lan, Wen Lei

Paper 183ag: Assembly and Processing of Titania Nanorods into Mesomorphic Ceramics

— **Mitchell Anthamatten**, Wenshi Zhang, Xinquan Cheng, Shaw H. Chen

MISC

Paper 183ah: First-Principles Study on the Electronic, Optical and Thermodynamic Properties of LaxSr, XCo, YFeyO₃-Δ (x/y =0.25, 0.5, 0.75) Perovskites

— **Ting Jia**, Paul R. Ohodnicki, Benajmin T. Chorpening, Gregory A. Hackett, Jonathan W. Lekse, Yuhua

Paper 183ai: Application of Hansen Solubility Parameter to Transparency Evaluation for Composite Materials — *Takahiro Nishida*, *Nobuyuki* Fujiwara, Shinichi Tsutsumi, Hideki

Paper 183aj: Modeling the Optical Properties of Silica Aerogel — *Hannah Margavio*

Yamamoto Sr.

Paper 183ak: Molecular Modifiers Reveal Unique Inhibition and Dissolution Mechanisms in Barite Scale

— **Ricardo D. Sosa**, Xi Geng, Jeremy C. Palmer, Michael A. Reynolds, Jacinta C. Conrad, Jeffrey D. Rimer

Paper 183al: Real Time Evaluation of Struvite Formation: Insights from the Macroscopic to Molecular Scale

— Doyoung Kim, Chara Olympiou,

Nicola Irwin, Jeffrey D. Rimer

Paper 183am: Direct Exfoliate Anode Graphite of Used Li-Ion Batteries into Few-Layer Graphene Sheets

— **Xifan Chen**, Yuanzhi Zhu, Wenchao Peng, Yang Li, Guoliang Zhang, Fengbao Zhang, Xiaobin Fan

Paper 183an: Effect of Material and Geometry of Nanofillers on Thermal Conductivity of Nanofluids — *Nitai Chandra Maji*, *Jayanta*

Paper 183ao: In-Situ Synthesis and Characterization of Mesoporous SBA-15 inside Enclosed Polymer Microchannels — Lani McKinnon, Hyeyoung Cho, Bonan Wang, Swomitra Mohanty, Jules Magda, Milind Deo, Michael Bartyl

Paper 183ap: Simple and Scalable Nanofabrication of Biomimetic Broadband Anti-Reflection Coatings on Silicon Wafers

— Peng Jiang

Chakrabortv

(184) Poster Session: Materials Engineering & Sciences (08E -Electronic and Photonic Materials)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Julianne L. Holloway, Chair Amy M. Peterson, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

Paper 184a: Design of FRET-Based Reversibly Photoswitchable Quantum Dot-DNA Conjugates

— **Thomas Porter**, Abhilasha Dehankar, Kil Ho Lee, Jessica O. Winter

Paper 184b: Single Iron Atoms Supported on MOF-Derived N-Doped Carbon for Robust Electrochemical CO₂ Reduction

— **Tingting Wang**, Bin Yang, Lecheng Lei, Yang Hou

Paper 184c: Tuning the Electronic and Structural Properties of MoS₂-Metal Interface through in-Silico Screening of Metal Contacts

— **Sagar Udyavara**, Ryan Wu, Rui Ma, Yan Wang, Manish Chhowalla, Turan Birol, Steven Koester, K. Andre Mkhoyan, Matthew Neurock

Paper 184d: Facile Solution Synthesis of Chalcogenide Perovskite Nanoparticles — *Alexander Jess, Brandon Partridge, Nicolas Macaluso, Charles Hages*

Paper 184e: Synthesis and Characterization of Nanoscale Europium Barium Titanate Eu_{0.5}Ba_{0.5}TiO₃
— Nasim Farahmand, Julien Lombardi, Frederick Pearsall, Zheng

Gai, Stephen O'Brien

(185) Poster Session: Materials Engineering & Sciences (08F -Composite Materials)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Julianne L. Holloway, Chair Amy M. Peterson, Co-Chair

Sponsored by: Materials Engineering and Sciences Division

MOF

Paper 185a: MOF-Derived Nanoparticles Coupled with N-Doped Porous Carbon Polyhedrons for Electrochemical Sensing

- Kaidong Wang, Guoqiang Jiang

Paper 185b: Understanding of *in-Situ* Growth of MOF in a Polymer Thin Film: Polyimide/ZIF-7 Mixed Matrix Membranes with Three Different Crystal Phases for Gas Separations

- Sunghwan Park, Hae-Kwon Jeong

Paper 185c: Computational Analysis of MOF-Enzyme Interactions for Next Generation of Sensitive Biosensors

— **Jordan Chapman**, Nagasree Garapati, Ahmed E. Ismail, Cerasela Zoica Dinu

■ WASTE RECOVERY

Paper 185d: Preparation of Ion-Imprinted Mesoporous Silica Functionalized with Aspargine for Adsorption of Nd(III) from Phosphogypsum Waste

— **Gebremedhn T. Gebremichael**, Grace M. Nisola, Rey Eliseo C. Torrejos, Lawrence A. Limjuco, Khino J. Parohinog, Hiluf Tekle Fissaha, Wook-Jin Chung

Paper 185e: Crown Ether Tethered on Silica Supports As Reusable Adsorbents for the Selective Capture of Cesium Ions in Water

— **Erwin C. Escobar**, Grace M. Nisola, Rey Eliseo C. Torrejos, Lawrence A. Limjuco, Khino J. Parohinog, Wook-Jin Chung

Paper 185f: Synthesis of Thermoresponsive Copolymer Immobilized on Silica Coated Magnetite and Its Application for Heavy Metal Ions Recovery

— **Hitoshi Tomonaga**, Kodai Hayashi, Junichi Ida, Tatsushi Matsuyama

Paper 185g: One-Pot Gamma Ray-Induced Green Synthesis of a Prussian Blue-Laden Aerogel for the Removal of Hazardous Pollutants

— **Go-Woon Lee**, Sung-Min Kang, Ji-Hee Kwon

COATINGS

Paper 185h: Conducting Polymer-Based Nanocomposite Anti-Corrosion Coatings for the Protection of Metals

— **Lekha Papammagari**, Sanjeev K Manohar, Adyant Shankar Paper 185i: Novel Polyoxometalatelonic Liquid with Antibacterial and Antifungal Properties. Feasibility of Its Implementation As a Multifunctional Thin Coating

— **Ana Enderle**, Isabel Franco Castillo, Mariela Bollini, Maria Julia Culzoni, Scott Mitchell, Carsten Streb

Paper 185j: Copper-Carbon Nanomaterial Based Composite Coatings for Dramatic Improvements in Pool Boiling Heat Transfer

— Aniket Rishi, Anju Gupta

MEMBRANES

Paper 185k: Quaternized g-Carbon Nitride—Polymer Nanocomposite Anion-Exchange Membranes

— **Joel Gaud**, Geovanna Santiago, Omar Móvil-Cabrera

Paper 1851: Two-Dimensional Porous Carbon Nanoplates Mixed Matrix Membranes for CO₂ Capture — Xiaochen Yang, Yan Dai, Weixin

Guan, Xuehua Ruan, Gaohong He
Paper 185m: Two-Dimensional

Nanochannel Membranes for Molecular and Ion Separations

— Leixin Yang, Shaofei Wang, Hong Wu**, Zhongyi Jiang**

Paper 185n: Ultrathin Membranes Based on Single-Layer Graphene and Laminar Graphene Oxide for Molecular Separation

— **Jing Zhao**, Feng Liang, Wanqin Jin

Paper 185o: PEO Based Composite Electrolytes Incorporating Lignocellulosic Nanofibrils for Solid-State Lithium-Ion Batteries

— Yidong Liu, Yong Min

Paper 185p: Facile Synthesis of Polymer/Magnetite Nanoparticle Composite

— **Kodai Hayashi**, Junichi Ida, Tatsushi Matsuyama

Paper 185q: Polyvinyl Alcohol (PVA) / Period 4-Based Ceramics Composites for Photovoltaic Applications

— **Natalie V. Duprez**, Kelsey E. Kohler, Kenneth L. Roberts

Paper 185r: Formulation of Photo Curable Resin for Highly Conductive 3D Printed Structures

— **Ling-Hsuan Chen**, Shang-Cheng Tsai, Ying-Chih Liao

Paper 185s: Melamine-Derived Graphene Foam As a Thermal Additive — *Emily Chase*, *Sungwoo Yang*

■ GENERAL COMPOSITES

Paper 185t: Mechanical Property Enhancement in Epon 862 Via Addition of Surface Modified Halloysite Nanotubes

— Edward W. Davis**, Haotian Wu**

Paper 185u: Granules Enable Multiscale Tissue-like Behaviors in Synthetic Hydrogels

— Yin Fang, Endao Han, Yiliang Lin, Yuanwen Jiang, Xianghui Xiao, Jin Wang, Heinrich M. Jaeger, Bozhi Tian Paper 185v: Interfacial Phenomena in Short Carbon Fiber Prepreg Manufacturing

— **Zachary Ř. Hinton**, Joy Baxter, Charleine Apangha Ngantsan, Maria M. Acevedo-Diaz, Simge Uzun, Prem Patel, Lavenia Thursch, Giuseppe Palmese, Nicolas J. Alvarez

Paper 185w: Thermo-Oxidative Aging Property of Polyurethane with Different Hindered Phenol Antioxidants

— **Quanxiao Dong**, Guanzhi Cheng, Yongjiang Xie, Xinguo Zheng, Shuming Li

Paper 185x: Observation of Oil-Film Formation in Gas-Assisted Gravity Drainage (GAGD) Using a Microfluidic Device

— **Kelly E. Robertson**, Shayan Sombolestani, Hannah C. Hymel, Jeffery C. Anderson, Dandina Rao, Adam T. Melvin

Paper 185y: Effects of Hydrocarbon Resins on the Performance of Silica-Filled Styrene-Butadiene Rubber and Butadiene Rubber Blend

— **De-yu Kao**, Ya-Chin Chen, Chih-Chen Hsieh, Chi-An Dai

(186) Poster Session: Nanoscale Science and Engineering

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Reginald E. Rogers Jr., Chair Micah J. Green, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

Paper 186a: Stooped Nanohairs with Randomized Configuration By Flood Electron Beam Under Ambient Pressure — Woojin Jung, Gyeon G. Jeon, Jung

— **Woojin Jung**, Gyeon G. Jeon, Jun H. Kim, Tae-il Kim

Paper 186b: Particle Atomic Layer Deposition of Yttrium Oxide for Hydrolysis Protection and Sintering of Aluminum Nitride Particles

— **Rebecca O'Toole**, Christopher J. Bartel, Christopher Gump, Charles B. Musgrave, Alan W. Weimer

Paper 186c: Quaternized g-Carbon Nitride As a High Performance Electrode Material for Supercapacitors

— **Rocio Lomba**, Shakira Martinez, Omar Movil-Cabrera

Paper 186d: Effects of Zeolite Dopant Atom Concentration on Noble Metal Nanoparticle Sintering Observed with *in Situ* UV-Vis Spectroscopy

— Elisha Converse, Steven C. Hayden, Huashan Li, Arthur France-Lanord, Jeffrey C. Grossman, Brian S. Hanna

Paper 186e: Ni²⁺—Modified g-Carbon Nitride Deposited on Carbon Fiber Paper for Supercapacitor Applications — Andrea Ramirez, Natalie De La Luz, Omar Móvil-Cabrera

Paper 186f: Engineering Xeno Nucleic Acid Nanosensors for Enhanced Stability — Alice J. Gillen, Justyna Kupis-Rozmysłowicz, Carlo Gigli, Nils Schuergers, Ardemis A. Boghossian Paper 186g: Thermo-Responsive lonophore Polymer Brushes Grafted on Magnetic Graphene Oxide As a Dual-Functional Composite Adsorbent for Selective Lithium Ion Recovery from Seawater

— Khino J. Parohinog, Hiluf Tekle Fissaha, Lawrence A. Limjuco, Grace M. Nisola, Wook-Jin Chung, Seong-Poong Lee

Paper 186h: DNA Reaction-Diffusion Attractor Patterns

— **Phillip Dorsey**, Dominic Scalise, Rebecca Schulman

Paper 186i: Near-Infrared Confocal Imaging of Single-Walled Carbon Nanotube Uptake in Bacterial Cells — Alessandra Antonucci, Vitalijs Zubkovs, Nils Schuergers, Ardemis A. Boghossian

Paper 186j: Characterization of Double-Stranded DNA on Single-Walled Carbon Nanotubes (SWCNTs)

— **Shang-Jung Wu**, Nils Schuergers, Kun-Han Lin, Alice J. Gillen, Clemence Corminboeuf, **Ardemis A. Boghossian**

Paper 186k: Impacts of a Low-Temperature Calcination on the Characteristics of Monodisperse, Surface-Clean, Supported Nanoparticle Catalysts

- Kristin Bryant, Steven R. Saunders

Paper 1861: MOFs Nanosheet Formation in Microreactor

— Kailin He**, Yingjian Luo**, King Lun Yeung

Paper 186m: Defect State Modulation of Wide Band Gap Semiconductor Nanoparticle for Potential Manifold Application

— **Tuhin Kumar Maji**, Debjani Karmakar, Samir Kumar Pal

Paper 186n: Fast and Green Microwave-Assisted Synthesis of Titania Nanotubes

— **Yingjian Luo**, Ana Serrano Lotina, King Lun Yeung, Miguel A. Bañares

Paper 1860: Bulk Synthesis of Quasi-Carbon Dot Via Two Step-Method from Rice Husk

— **Prashant Kumar**, Sudipto Chakraborty

Paper 186q: Polyacrylonitrile and Polypropylene Carbonate Blended Solid Polymer Electrolytes for Application Toward Solid State Lithium Ion Batteries — Jed LaCoste, Saraj Banjara, Drew Matherne, Zizhou He, Ling Fei

Paper 186r: Real-Time Evaluation of Cellular Behavior upon Exposure to Metallic Organic Frameworks

— **Olivia Rose**, Alixandra Wagner, Qian Liu. Cerasela Zoica Dinu

Paper 186s: Sequence and Aggregation State Determine Stability, Endosomal Processing and Long-Term Fate of DNA-Wrapped Carbon Nanotubes in Mammalian Cells

— **Mitchell Gravely**, Mohammad Moein Safaee, Daniel Roxbury Paper 186t: Light Absorption from Gold Nanoparticle Agglomerates

— **Georgios A. Kelesidis**, Daniel Gao, Sotiris E. Pratsinis

Paper 186u: Ion-Induced Nucleation of Carbonaceous Nanoparticles

— **Kimberly Bowal**, Jacob W Martin, Laura Pascazio, Markus Kraft

Paper 186v: Nanowire Organic Sensor for Ammonia Detection

— **Mohamed Kilani**, Xuecheng Yu, Guangzhao Mao

Paper 186w: Bandgap Engineering of 2D Metal Oxides Using Sulfur for Catalytic and Electronic Applications

— **Nikita Sugak**, Matthew Montgomery, Facheng Guo, Yulian He, Lisa Pfefferle, Victor S. Batista

Paper 186x: Synthesis and Separation of Metallic Nanoparticles in Aqueous Two Phase System

— **Krishna Vadiraj Kinhal**, Shashwata Sinha, Aishwarya R, Nirav Bhatt, Subramanium Pushpavanam

Paper 186y: Facile Method to Fabricate Nanostructured Silver Selenide Thin Films at Room Temperature from a Copper Selenide Template

— **Nan (Louise) Chen**, Michael Scimeca, Peter Zhao, Ayaskanta Sahu

Paper 186z: Diffusion of Species in Functionalized Micro/Mesoporous Au@ SiO₂ Core-Shell Nanoparticles

— **Ellis Hammond-Pereira**, Steven R. Saunders

Paper 186aa: An Ion Redistributor for Dendrite-Free Lithium Metal Anodes

— **Chen-Zi Zhao**, Peng-Yu Chen, Rui Zhang, Xiang Chen, Bo-Quan Li, Xue-Qiang Zhang, Xin-Bing Cheng, Qiang Zhang

Paper 186ab: Mediatorless, Reversible Optical Nanosensor Enabled through Enzymatic Pocket Doping

— **Vitalijs Zubkovs**, Nils Schuergers, Benjamin Lambert, Esra Ahunbay, Ardemis A. Boghossian

Paper 186ac: Spinning-Disc Confocal Microscopy in the Second Near-Infrared Window (NIR-II)

— Vitalijs Zubkovs, Alessandra Antonucci, Nils Schuergers, Benjamin Lambert, Andrea Latini, Raino Ceccarelli, Andrea Santinelli, Andrii Rogov, Daniel Ciepielewski, Ardemis A. Boghossian

Paper 186ad: Accumulative Roll Bonding (ARB)-Processed High-Manganese Twinning Induced Plasticity (TWIP) Steel with Extraordinary Strength and Reasonable Ductility

— Arash Etemad

Paper 186ae: Engineering Ionically-Gelled Chitosan Nanoparticles Containing the Nucleoside Analog, Gemcitabine

- Austin Fergusson, Richey M. Davis

Paper 186af: The Effects of Scavenger Receptor Class B Type 1 on the Uptake of Both Hard and Soft Nanoparticles — Mitch Raith, Uche Anozie, Paul Dalhaimer

Paper 186ag: Process Intensification for Small Molecule Synthesis Via Recombinant Peptide Templated Palladium and the Elimination of Intermediate Purification

— **Imann Mosleh**, M. Hassan Beyzavi, Robert Beitle

Paper 186ah: A Shapelet-Based Method for Analysis of Self-Assembled Surface Imaging

— Thomas J. Akdeniz, **Nasser M. Abukhdeir**

Paper 186ai: Reorientation Dynamics and Symmetry-Breaking of Confined Nematic Liquid Crystal Domains — Fu Fred, Nasser M. Abukhdeir

Paper 186aj: Hierarchical Zeolite Templated-Carbon Materials for Clean Energy Applications

— Marie Bermeo, Lourdes F. Vega, Mohammad Abu Zahra, Maryam Khaleel

Paper 186ak: Metal-Encapsulated Carbon Nanotubes to Enhance Dispersion in Metal Matrix Composites — Gregory E. Chester, Anna P. Skinner, Kirk J. Ziegler, Justin J. Hill

Paper 186al: Reengineering the Tumor Microenvironment to Enhance Nano-Immunotherapy

— John D. Martin

Paper 186am: Advanced Removal / Extraction of the Hydrocarbons by Emulsion Liquid Membrane Enhanced by Nanoparticles

— **Qusay Al-Obaidi**, Muthanna Al-Dahhan

(187) Poster Session: Next-Gen Manufacturing

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Nima Yazdanpanah, Chair Ignasi Palou-Rivera, Co-Chair

Sponsored by: Next-Gen Manufacturing

Paper 187a: Modeling Rosette
Nanotubes for Applications in Water
Filtration, Biosensing and Drug Delivery
— Vyshnavi Karra, Prabhat Tirpathi,
Meni Wanunu, Sidi Bencherif, Hicham
Fenniri, Francisco R. Hung

Paper 187b: Enhancing Tractability of Model Predictive Control-Assisted Online Data Collection — *Henrique Oyama*, *Helen Durand*

Paper 187c: Model-Guided Design of

a Solar-Assisted Water Desalination Process through Membrane Distillation — *Mahdi Mohammadi Ghaleni*, Abdullah Al Balushi, Mona Bavarian, Siamak Nejati Paper 187d: Multiscale Modeling of Pulp Fiber Length in Batch Pulping Process — *Hyun-Kyu Choi*, *Joseph Sang-Il Kwon*

Paper 187e: FDM of ABS-Nanoclay Composites

— **Burcin Ikizer**, Azadeh Farahanchi, Nese Orbey

Paper 187f: Experimental Modeling of a Nonlinear Hybrid Dynamic System — Hainan Wang, Edward P. Gatzke

Paper 187g: A Workflow for the Fabrication of Innovative Crystallizers Using 3D-Printing

— **Kiran Mathew Thomas**, Richard Lakerveld

Paper 187h: Thermal Effects on Capillary Flow in Polymeric Powders — Katrina J. Donovan, James Stasiak, Willie E. "Skip" Rochefort, Garry Hinch

Paper 187i: An Advanced 3D
Computational Model for Designing
Next Generation Drug Carriers
— Abdollah Koolivand, Panagiotis
Dimitrakopoulos

Paper 187j: 3D Printing and Robotic Filling of Multi-Compartment Capsular Devices for Oral Drug Delivery

— Alice Melocchi, Federico Parietti

Paper 187k: Material Extrusion Based Additive Manufacturing with Blends of Polypropylene and Hydrocarbon Resins — Arit Das, Alexandra Marnot, Eugene G. Joseph, Michael J. Bortner

Paper 1871: Effect of Temperature on the Morphology of Extruded Strand in Fused Deposition Modeling: A CFD Study

— **Behrouz Behdani**, Leah Mason, Ming Leu, Joontaek Park

Paper 187m: Process Intensification in Solid Dosage Formulation By Hot Melt Extrusion

— José Hernández Espinell, Francheska M. Reyes Figueroa, Vilmalí López-Mejías, Torsten Stelzer

(188) Poster Session: Novel Products from Forest and Plant Biomass

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S Shri Ramaswamy, Chair

Sponsored by: Forest and Plant Bioproducts Division

Paper 188a: Filament Fabrication and 3D Printability of Poly(3hydroxybutyrate-co-3-hydroxyvalerate) (PHBV)/Poly(lactic acid) (PLA) blends using a Commercial Chain Extender — Miguel A. Vigil Fuentes, Suman

— Miguel A. Vigil Fuentes, Suman Thakur, Manju Misra, Stefano Gregori, **Amar K. Mohanty**

Paper 188b: Evaluation of Binderless Board Made from Composted Rice Straw As Substrate for Rice Seedling Production

— Ping Qu

Paper 188c: A Closed-Loop Biorefinery for Woody Biomass Conversion Using Lignin-Derived Deep Eutectic Solvents - Yunxuan Wang, Xianzhi Meng, Yunqiao Pu, Kwang Ho Kim, Arthur J. Ragauskas, Chang Geun Yoo

Paper 188d: Reuse of Sustainable Wastes for Fibreboard Production: The Case of Waste Paper and Water Hyacinth

- Ebenezer Ojo, Festus Oyawale

Paper 188e: Polyhydroxyalkanoate and Cellulose Ester Based Biodegradable Plastic Blends for Sustainable Packaging - Kjeld Meereboer, Akhilesh K. Pal, Amar K. Mohanty, Manju Misra

Paper 188f: Extraction of Eucalyptus Globulus Leaves with Distinct Methods and Solvents. Comparison and Analysis of the Extracts

- Vitor H. Rodrigues, Marcelo M.R. de Melo, Vico Tenberg, Jose P. S. Aniceto. Rui Carreira, Inês Portugal, Carlos M.

(189) Poster Session: Pharmaceutical Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

Shujauddin M. Changi, Chair **Christine Seymour, Co-Chair**

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

Paper 189a: A Comprehensive Sensitivity Analysis for Risk Assessment of a Pharmaceutical Crystallization Process Merve Öner, Stuart Michael Stocks, Jens Abildskov, Gürkan Sin

Paper 189b: Advancing from QbD to Operational Excellence in Continuous Pharmaceutical Manufacturing

— **Sudarshan Ganesh**, Benjamin Rentz, Le Bao Dan Vo, Zoltan K. Nagy, G. V. Rex Reklaitis

Paper 189c: Application of Life-Cycle Concepts in Drug Substance Manufacturing

— Ajay Babu Pazhayattil, Marzena

Paper 189d: Establishing Meaningful Alarm Limits for a Continuous Direct Compression Process

- Jenna Brandon

Paper 189e: Assessment of Blend Uniformity in a Continuous Tablet Manufacturing Process

Nobel O. Sierra-Vega, Rafael Méndez-Román

Paper 189f: Continuous Pharmaceutical Manufacturing of Uniform Crystals in Slug Flow

— Mingyao Mou, Huayu Li, Bing-Shiou Yang, Mo Jiang

Paper 189q: Experimental Analysis of Influence Screw Configuration in View of Understanding Granulation Mechanism in Pharmaceutical Twin-Screw Melt Granulation

- Shana Van de Steene, Jeroen Van Renterghem, Chris Vervaet, Thomas

Paper 189h: How a Material Property Library Can Promote Rapid Process Development

– James V. Scicolone, Fernando J. Muzzio

Paper 189i: Agitator Impact on the Net Weight Signal of a Loss-in-Weight Feeder Operating at Low Mass Flow Rates

— Marcus O'Mahony, Steven Dale, Eric Dinarello, Ian Kinney, Hudson Gloria, Greg Connelly

Paper 189j: Temperature Mapping of Pharmaceutical Trickle Bed Reactor for Continuous Hydrogenation

- Huibo Sheng, Tomislav Ljubicic, Angel Diaz, David Pfisterer, Joel M. Hawkins, Jason Mustakis

Paper 189k: In-Line NIR Spectroscopy for Monitoring the Preparation of Ginkgo Biloba Extract Solid Dispersions By Hot-Melt Extrusion

- **Luming Liu**, Haibin Qu

Paper 1891: Filtration Studies Combined with Mechanistic Modelling to Reliable API Process Understanding and Scale-up

- Rui Pina Campos, Filipe Ataíde, Ana Cruz, Emília Leitão, Rui Loureiro

Paper 189m: Filtration Process Modeling and Scale-up for Robust Drug Substance Manufacturing

- Wenbin Hu, Carlos Orihuela, Jace Fogle

Paper 189n: Forget Throughput, It's about the Risk- Rethinking Dead-End Membrane Filtration Scale-up - Kelly Wei

Paper 189o: Development of an

Expanded Parametric PBE Using Experimental Data from a High Shear Wet Granulation Process

Carlos Velazquez, Madeline Candelaria, Luis F. Torrens-Sotomayor

Paper 189p: A Chemical Engineering Approach to Modelling Drug Dissolution and Transport Phenomena in the Lower **Gastrointestinal Tract**

- Connor O'Farrell, Konstantinos Stamatopoulos, Eva M. Karlsson, Luca Marciani, Sarah Sulaiman, Hannah K. Batchelor, Mark Simmons

Paper 189q: Optimizing the Pharmaceutical Cleaning Process: Challenges and Opportunities

- Rabah Mouras, Gavin Walker, Ahmad B. Albadarin

Paper 189r: The Development of a 2-Step Buprenorphine Intermediate 5 **Process**

- Wen-Chun Zhang

Paper 189s: Arginine Interactions Resulting in Virus Inactivation

— Christa Meingast, Pratik U. Joshi, Caryn L. Heldt

Paper 189t: Once Weekly Oral Ivermectin for Prevention of Malaria Transmission in Zone IVb

— **Juna Yana**. Rosemarv Kanastv. Susan Low, Tyler Grant, Juan Jaramillo Montezco, Sonia Holar, Deblina Biswas, Adam Habshev

Paper 189u: Characterization of the Formulation-Process Interaction for Improved Thermal Bonding in the Manufacture of a Novel Ultra-Long Acting Oral Dosage Form

- Sonia Holar. Juan Jaramillo Montezco, David Dufour, Susan Low, Kristie Sykes, Rose Kanasty, Tyler Grant

Paper 189v: Development of pH -Responsive Disintegrating Matrices for Safe Intestinal Transit of Gastric Resident Dosage Forms

— **Juan Jaramillo Montezco**, Sonia Holar, Jung Yang, Marlene Schwarz, Kristie Sykes, Susan Low, David Alteruter, Tyler Grant, Rose Kanasty, Andrew Bellinger

Paper 189w: Single-Use Centrifuge for Large Scale Separation and Collection of CHO and mAbs, and Other Cell Culture Applications

- David R. Richardson

Paper 189x: Solubility Enhancement of Hydrophobic Drug Molecules Via Amorphous Solid Dispersions and Flash Nanoprecipitation

- Nicholas J. Caggiano, Robert K. Prud'homme, Rodney D. Priestley

Paper 189y: Comparison of Oral Drug Dissolution between Medium and Long Chain Unsaturated and Saturated Triglycerides: A Modeling-Based Approach

Bhavya Singh

Paper 189z: Enhancing the Long-Term Storage Stability of Amorphous Drug-Polyelectrolyte Nanoparticle Complex Via Incorporation of Hypromellose

— Kunn Hadinoto, Chew Jia Wei

Paper 189aa: Understanding Polymorphic Phase Transformations of Acetaminophen in Polymer-Based Formulation Processes

José Hernández Espinell, Betsy Orta, Vilmalí López-Mejías, Torsten Stelzer, Giovanni López Burgos

Paper 189ab: Application of Artificial Neural Network As a Predictive Tool for Continuous Liposome Processing

- Sameera Sansare, Hossein Mohammadiarani, Antonio Costa, Xiaoming Xu, Celia N. Cruz, Su-Lin Lee, Diane Burgess, Bodhisattwa Chaudhuri

Paper 189ac: Development of a Blistering Packaging Process with Nitrogen-Modified Headspace

— Margaret R. Dowst, Niranjan S. Kodgule, Jennifer M. Vandiver, Mark Oliveira, Michael Young, Mark Tawa, Erica Connolly

Paper 189ad: Dropwise Additive Manufacturing for Pharmaceuticals — Andrew J. Radcliffe, Zoltan K. Nagy, Gintaras V. Reklaitis

Paper 189ae: Buckling of a Drying . Colloidal Drop

— Mahesh S. Tirumkudulu

(190) ABET Updates and Insights (Invited Talks)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 22 Randy S. Lewis, Chair **Douglas Ludlow, Co-Chair**

Sponsored by: Undergraduate Education

3:30 Introductory Remarks

4:30 Panel Discussion

(191) Adsorption Applications for **Sustainable Energy and Chemicals** Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Manatee Spring II

F. Handan Tezel, Chair

Sponsored by: Adsorption and Ion Exchange

3:30 Paper 191a: Adsorption of Fluoroguinolones at Gas-Liquid Interface By Foam Fractionation

- Rajesh Ghosh, Haritha Hareendran, Subramanium Pushpavanam

3:50 Paper 191b: Sorbent Enhanced Reverse Water Gas Shift Reaction: Maximizing CO Yield

- Johannis A. Z. Pieterse

4:10 Paper 191c: Modeling and Optimization of a Moving Bed Process for Post-Combustion CO, Capture Using a Diamine-Appended Metal-Organic Framework

- **Ryan Hughes**, Goutham Kotamreddy, Debangsu Bhattacharyya, Michael S. Matuszewski, Benjamin P. Omell, Jeffrey R. Long, Rebecca Siegelman, Stephanie Didas, Surya Parker

4:30 Paper 191d: Separation and Purification of Bioderived Furanic Molecules with Metal-Organic Frameworks

 Yadong Chiang, Ryan Lively, Sankar Nair

A. Valla

4:50 Paper 191e: Investigation of Rare Earths Exchanged on Zeolite Y for Adsorptive Desulfurization of Model Fuels in the Presence of Aromatics - Tyler B. Crowl, Kevin X. Lee, Julia

5:10 Paper 191f: Catalytic Adsorptive Desulfurization of Model Fuel over Ti-Si Adsorbents at Low Ti Loading Under **Ambient Conditions**

— Xiong Dai, Guang Miao, Liqiong Wu, Zhong Li**, Jing Xiao**

5:30 Paper 191g: Desulfurization of Fuels Using Activated Carbon Prepared from Asphaltenes

Efstratios Svinterikos, Ioannis Zuburtikudis, Mohamed Al Marzougi

(192) Advanced Combustor Concepts Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Challenger 40 Ron Breault, Chair

Sponsored by: Advances in Fossil **Energy R&D**

- 3:30 Paper 192a: NO Emissions for Rotating Detonation Combustion Operating on Hydrogen-Air and Hydrogen/Natural Gas - Air
- Donald Ferguson, Arnab Roy, Pankaj Saha, Peter Strakey, Todd
- 3:48 Paper 192b: Recent **Developments in Colorless Distributed** Combustion (CDC)
- Ashwin Gupta

Scott Martin

- 4:06 Paper 192c: Ultrasonic Measurements of Temperature Distribution and Heat Flux Vectors in Solid Components of Energy Conversion Processes
- Yunlu Jia, Mikhail Skliar
- 4:24 Paper 192d: CFD Simulations of Propane/Natural Gas Blended Fuels Combustion in Gas Turbine
- Yong Liu, Mehrdad Shahnam, Chris Guenther
- 4:42 Paper 192e: Advanced Oxy-Combustor Concepts for Direct-Fired Supercritical CO₂ Power Cycles - Subith Vasu, K.R.V. Manikantachari,
- 5:00 Paper 192f: Pressurized Oxy-Fuel Combustion in Fluidized Bed: 3D CFD Simulation with Experiment
- Jinrao Gu, Yingjuan Shao, Wengi Zhong
- 5:18 Paper 192g: Experimental Study of SO, Emissions and Desulfurization of Oxy-Coal Combustion in a Pressurized Fluidized Bed Combustor
- Lei Pang, Wengi Zhong, Yingjuan
- 5:36 Paper 192h: Assessment of Oxy-Fuel Combustion System with Coal and Biomass Co-Firing Based on Circulating Fluidized Bed
- Yan Shi, Qinwen Liu, Yingjuan Shao, Wenqi Zhong

(193) Advances in Machine Learning **Methods for Process Systems Engineering**

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 26 Zhenyu Wang, Chair Qi Zhang, Co-Chair

Sponsored by: Data and Information

- 3:30 Paper 193a: Smart Process Data Analytics: Automated and Robust Data Analytics for Manufacturing Processes Weike Sun, Richard D. Braatz
- 3:49 Paper 193b: How Does a Deep Neural Network Learn to Approximate Functions?
- Abhishek Sivaram, Laya Das, Venkat Venkatasubramanian

- 4:08 Paper 193c: When Have Two Networks Learned the Same Task? Data-Driven Transformations between System Representations
- Tom S. Bertalan, Felix Dietrich, Thomas Thiem, Ioannis G. Kevrekidis
- 4:27 Paper 193d: Machine Learning through a Parametric Programming Lens - William W. Tso, Baris Burnak, Melis Onel, Justin Katz, Efstratios N. Pistikonoulos
- 4:46 Paper 193e: A New Tool for Selection Surrogate Modeling Technqiues for Design Space Approximation and Surrogate-Based Optimization
- Bianca Williams. Selen Cremaschi
- 5:05 Paper 193f: Parametric Surrogate Model Generation Using Adaptive Sparse Grid Interpolation
- Chris Kieslich, Fani Boukouvala
- 5:24 Paper 193q: Physics-Aware Machine Learning Algorithms with Improved Accuracy and Explainability Applied to Multiphase Flowrate Estimation
- Timur Bikmukhametov Johannes
- 5:43 Paper 193h: Online Adaptive Sparse Identification of Systems (OASIS): Application to CSTR
- Bhavana V.N.S. Bhadriraju, Abhinav Narasingam, Joseph Sang-Il Kwon

(194) Advances in Optimization: Global, Uncertainty, Surrogate & Mixed-Integer Models I

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 24 John D. Siirola, Chair Pedro M. Castro, Co-Chair

Sponsored by: Computers in **Operations and Information Processing**

- 3:30 Paper 194a: Admm Preconditioning for Block-Structured Linear Algebra Systems
- Jose Rodriguez, Carl Laird, Victor M. Zavala
- 3:49 Paper 194b: Easily Solvable Convex Mixed-Integer Nonlinear Programs Derived from Generalized Disjunctive Programming Using Cones
- David E. Bernal, Ignacio E. Grossmann
- 4:08 Paper 194c: Quantum Computing Based Hybrid Quantum-Classical Solution Approach for Complex **Combinatorial Optimization Problems**
- Akshay Ajagekar, Fengqi You
- 4:27 Paper 194d: Reachability Bounds for Global and Robust Optimization of Parametric ODEs Via Implicit Methods
- Matthew Wilhelm, Matthew D. Stuber
- 4:46 Paper 194e: Nested Decomposition Algorithms for Large-Scale Multi-Period and Multistage Stochastic Mixed-Integer Linear **Programming Models**
- Ignacio E. Grossmann, Cristiana L. Lara

- 5:05 Paper 194f: An Interior-Point I,-Exact Penalty Strategy for Degenerate Nonlinear Programming Problems within IPOPT
- David Thierry, Lorenz T. Biegler
- 5:24 Paper 194g: Variable Bounds Tightening for Nonconvex MINLP with Application to Multiperiod Blending - Yifu Chen. Christos T. Maravelias
- 5:43 Paper 194h: Model Reduction-Based Global Optimisation for Large-Scale Steady State Nonlinear Systems - Min Tao, Constantinos Theodoropoulos

(195) Applications of Data Science in Molecular Sciences I

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Peacock Spring **Andrew White, Chair** Andrew L. Ferguson, Co-Chair Johannes Hachmann, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

- 3:30 Paper 195a: Multi-Objective, Machine-Learning Assisted First-Principles Design of Transition Metal Complexes for Redox Couples — **Jon Paul Janet**, Heather J. Kulik
- 3:45 Paper 195b: Machine Learning the Fundamental Tradeoffs between Conductivity and Voltage Stability in Solid State Electrolytes
- Karun K. Rao, Michael Nikolaou, Yan Yao, Lars C. Grabow
- 4:00 Paper 195c: Machine Learning for the Prediction of Electronic Couplings and Charge Transport Calculations in PaHT - Eric Jankowski
- 4:15 Paper 195d: Endotoxin Sensors Using Liquid Crystals and Machine Learning
- Shengli Jiang, Junghyun Noh, Alexander Smith, Nicholas L. Abbott, Victor M. Zavala
- 4:30 Paper 195e: Microscopic Modeling and Optimal Operation of Thermal Atomic Layer Deposition - Yichi Zhang, Yangyao Ding, Zhe

Wu, Panagiotis D. Christofides

- 4:45 Intermission
- 5:00 Paper 195f: Thermodynamic Properties Via a Combined Expanded Wang-Landau - Machine Learning Approach
- Caroline Desgranges, **Jerome Delhommelle**
- 5:15 Paper 195g: Understanding Mixing Behavior of Bimetallic Nanoparticles through Genetic Algorithm Modeling
- Michael Cowan, James Dean, Giannis Mpourmpakis
- 5:30 Paper 195h: Estimation of Probability Density Functions of Model Parameters for a Heterogeneous Population with Neural Network: Application to TNFα Signaling Pathway - Dongheon Lee, Arul Jayaraman, Joseph Sang-II Kwon

- 5:45 Paper 195i: Development of Multimodal Cancer Diagnosis Method Based on Medical Image Analysis and Raman Spectroscopy
- **Jian-Hao Li**, Inge K. Herrmann

(196) Catalysis with Microporous and Mesoporous Materials III: Material Design

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Florida Ballroom A Marat Orazov, Chair

Iman Noshadi, Co-Chair

Sponsored by: Catalysis and Reaction **Engineering Division**

- 3:30 Paper 196a: Micro/Mesoporous Au@SiO, Core-Shell Nanoparticles for Alkalinity-Independent Selective Benzyl Alcohol Oxidation
- Ellis Hammond-Pereira, Kristin Bryant, Trent R. Graham, Steven R. Saunders, Di Wu
- 3:50 Paper 196b: Evaluating Catalytic Activity for Hierarchical Beta Zeolites: The Effect of Mesopore Configuration and Synthetic Strategy
- **Ke Zhang**, Elisha Converse, Sergio Fernandez, Michele L. Ostraat
- 4:10 Paper 196c: Fin-like Zeolite Crystals: A New Class of Hierarchical Catalysts
- **Heng Dai**, Yufeng Shen, Donglong Fu, Thuy T. Le, Taimin Yang, Matthias Filez, Xiaodong Zou, Bert M. Weckhuysen, Jeffrey D. Rimer
- 4:30 Paper 196d: First-Principles Investigation of Cu Ion Exchange and Siting Preference in FER Zeolite
- Sichi Li**, Zhenghang Zhao**, Yujia Wana, Casev Jones, John R. Di Iorio, Anthony DeBellis, Subramanian Prasad, Ahmad Moini, Rajamani Gounder, William F. Schneider
- 4:50 Paper 196e: Identification of Distinct Sn Sites in Siliceous Zeolites for Mpvo and C-C Bond Formation Catalysis - **John R. Di Iorio**, Jennifer Lewis, Yuriy Román-Leshkov
- 5:10 Paper 196f: Synthesis of Bifunctional Zeolite-Encapsulated Metal Nanoparticles with Intimacy between Metal and Acid Sites for Tandem
- Hong Je Cho, Bingjun Xu
- 5:30 Paper 196g: Polymer-Nanocrystal Hybrid Catalysts Demonstrate Control of Transition State and Product Diffusion - Andrew Riscoe, Cody Wrasman, Andrew A. Herzing, Adam Hoffman, Aditya Menon, Alexey Boubnov, Simon R. Bare, Matteo Cargnello

(197) Chemical and Catalytic Conversions and Processes for Renewable Feedstocks

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom T

Michael Mullins, Chair Aida Amini Rankouhi, Co-Chair

Sponsored by: Sustainable Biorefineries

- **3:30 Paper 197a:** Conversion of Cellulose and Amino Acids to High-Value-Added Chemicals Using Saturated Steam
- **Seiichiro Yoshida**, Keiichiro Matsushima, Tohru Joboji
- **3:55** Paper **197b**: Non-Thermal, Atmospheric Plasma Conversions of Biomass into Value-Added Chemicals: Solvent-Plasma Based Conversion *Lusi A, Xianglan Bai, Hui Hu*
- **4:20 Paper 197c:** Treatment of Biomass Gasification Tars with Non-Thermal Plasmas
- **Faisal Saleem**, Kui Zhang, Adam P. Harvey
- **4:45** Paper **197d**: Upgrading of Biorenewable Thermal Deoxygenation Oils to Aviation Fuel Range Hydrocarbons
- Sampath A. Karunarathne, Matthew J. Kline, M. Clayton Wheeler
- **5:10 Paper 197e:** A Comparative Study on Chemical Kinetic Models for the Biomass Pyrolysis Reactions
- Karen A Izumida, **Joao G. R. Poco**, Ronaldo Santos
- **5:35 Paper 197f:** Mesoporous Metal Oxide Aerogels for Sustainable Fuels Generation
- **Ashley M. Pennington**, Catherine L. Pitman, Paul A. DeSario, Jeremy J. Pietron, Todd H. Brintlinger, Debra R. Rolison

(198) Crystallization of Pharmaceutical and Biological Molecules

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Coral Spring I/II Venkateswarlu Bhamidi, Chair Manish S. Kelkar, Co-Chair Joshua Engstrom, Co-Chair

Sponsored by: Crystallization and Evaporation

- 3:30 Welcoming Remarks
- **3:33 Paper 198a:** Screening of Polymorphs and Measurement of Growth Rates of L-Histidine at Controlled Supersaturation Using Continuous-Flow, Microfluidic Device
- **Paria Coliaie**, Manish S. Kelkar, Nandkishor Nere, Meenesh R. Singh
- **3:53 Paper 198b:** Homogeneous Nucleation and Size Distributions of Protein Crystals Nucleated and Grown in Weightlessness
- Paul W. Todd, Michael Sportiello

- **4:13** Paper 198c: A New Molecular Templating Approach for Controlling the Nucleation of Peptides
- Frederik J. Link, Jerry Y.Y. Heng
- **4:33 Paper 198d:** Measuring the Rate of Co-Crystal Nucleation Utilizing Continuous Microfluidic Droplet Generation
- Scott Pedu, Shelley L. Anna
- **4:53 Paper 198e:** Impacts of Solvent and Polymer Additive Polyvinylpyrrolidone on the Ethyl Vanillin Crystal Morphology
- **Shihao Zhang**, Ling Zhou, Chuang Xie, Baohong Hou, Qiuxiang Yin
- **5:13 Paper 198f:** Impact of Polymers and Surfactants on Solid-State Crystallization at the Amorphous Pharmaceutical-Water Interface
- **Andrew S. Parker**, Lynne S. Taylor, Stephen P. Beaudoin
- **5:33 Paper 198g:** Continuous Protein Crystallization in a 3D Printed Airlift Crystallizer
- Kiran Mathew Thomas, Yi Jin, Richard Lakerveld

(199) Data-Driven Techniques for Dynamic Modeling, Estimation, and Control I

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 25 Kirti M. Yenkie, Chair Daniel Chen, Co-Chair

Sponsored by: Systems and Process Control

- **3:30 Paper 199a:** Fast and Large-Scale Model Predictive Control Using Neural Networks
- **Pratyush Kumar**, James B. Rawlings
- **3:48** Paper 199b: Data Driven Plant Model Mismatch Estimation for Dmc with Unknown Noise Variance
- **Xiaodong Xu**, Jodie Simkoff, Michael Baldea, Leo H. Chiang, Rahul Bindlish, Ivan Castillo
- **4:06** Paper 199c: Model Predictive Control of Phthalic Anhydride Synthesis in a Fixed-Bed Catalytic Reactor Via Machine Learning Modeling
- **Zhe Wu**, Anh Tran, Yi Ming Ren, Scarlett Chen, Panagiotis D. Christofides
- **4:24** Paper 199d: Data-Driven Design of Hierarchical MPC Architectures
- Ranjeet Kumar, **Victor M. Zavala**
- **4:42** Paper **199e:** Integrating Data Driven Modeling with First Principles Knowledge
- Nikesh Patel, Jake Nease, Siam Aumi, Christopher Ewaschuk, Jie Luo, Prashant Mhaskar
- **5:00** Paper 199f: Optimal Control for Simulated Moving Bed Process with Deep Reinforcement Learning
- Tae Hoon Oh, Jong Min Lee
- **5:18** Paper 1999: Input Design for Active Fault Diagnosis: Recent Developments, New Results, and Future Directions
- Tor Aksel N. Heirung, Ali Mesbah

5:36 Paper 199h: Improving Near-Infrared Spectrum-Based Soft Sensor Performance through Variable Selection — Jangwon Lee, Jin Wang, Q. Peter He

(200) Design, Analysis, and Optimization of Sustainable Energy Systems and Supply Chains III

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom V

Dharik Mallapragada, Chair Fengqi You, Co-Chair Zuwei Liao, Co-Chair

Sponsored by: Sustainable Energy

- **3:30** Paper 200a: Incorporation of Network Topology for Resilient Design and Optimal Operation in the Framework of Water-Energy Nexus *Spyridon D. Tsolas, M. Nazmul*
- **3:55 Paper 200b:** Innovative Processes Design for Value-Added Products from Natural Gas Liquids in Shale Gas

Karim, M. M. Faruque Hasan

- **Yiru Li**, Zewei Chen, Edwin Andres Rodriguez Gil, Rakesh Agrawal
- **4:20 Paper 200c:** Optimal Design of Flowsheets Via Surrogate-Based Sub-Process Models: A Case Study of CO₂ Capture and Utilization
- **Zhimian Hao**, Polina Yaseneva, Alexei A. Lapkin
- **4:45** Paper **200d**: Techno-Economic Analysis (TEA) of CO₂ Electrolysis Systems for Ethylene Production
- **Wenqin Li**, Victor Beck, Jeremy T. Feaster, Sarah E. Baker, Eric B. Duoss
- **5:10** Paper 200e: Nutrient Pollution Prevention By Implementing Nutrient Recovery Technologies in Livestock Facilities
- **Edgar Martín-Hernández**, Apoorva Sampat, Mariano Martín, Victor M. Zavala, Gerardo J. Ruiz-Mercado

(201) Developments in Petroleum and Biofuels Refining Technologies

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Challenger 38/39

Robert Sigal, Chair Dongting Zhao, Co-Chair YuJeng Lin, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

- **3:30** Paper 201a: Improvement of Transportation Fuels Sustainability Via Co-Hydroprocessing of Lipid-Feedstocks and Petroleum Fractions
- **Stella Bezergianni**, Athanasios Dimitriadis, Loukia Chrysikou, Vasilios Dimitropoulos, Maria Maggiliotou, Spyridon Kiartzis, Spyridon Voutetakis
- **3:51** Paper 201b: Pyrolysis of Solid Food Court Waste Mixtures Coupled with *Ex-Situ* Catalytic Upgrading *Gabriela Ionescu, Razvan N. State,* **Dorin Boldor,** Cosmin Marculescu

- **4:12 Paper 201c:** In-Situ Evaluation of the Concentration of 1-Hexene in a Laboratory-Scale Fluid Catalytic Cracking (FCC)
- Juan Lacayo, David Soto, Sebastian López, **Alejandro Molina Ochoa**
- **4:33 Paper 201d:** Development of Rigorous Refining Simulation Models to Determine Greenhouse Gas Emission Impact of Canadian Crude Oil Bends in a Refinery
- **Abayomi Oni**, Eskinder Gemechu, Amit Kumar
- **4:54** Paper 201e: Suitable Characteristics for Surfactants Substituent of Antifoam Silicon Oil *Rafael F. Perez, Osvaldo Karnitz Jr., João B. V. S. Ramalho, Claudia E.*
- Mansur
 5:15 Paper 201f: Impact of Deep
 Hydrogenation on Jet Fuel Oxidation
- and Deposition
 Tinghao Jia, Lun Pan, Ji-Jun Zou, Li
 Wang, Xiangwen Zhang

(202) Distillation: Recent Developments in Advanced Techniques and Process Intensification

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Barrel Spring II Andrew W. Sloley, Chair

Sponsored by: Distillation and Absorption

- 3:30 Welcoming Remarks
- **3:32 Paper 202a:** Optimal Design and Control of Reactive Distillation Systems Under Uncertainty
- Aikaterini Tsatse, Stijn Oudenhoven, Antoon ten Kate**, Eva Sorensen**
- **3:55** Paper 202b: Phase Equilibria of a Reactive Distillation Process for Isobutyl Acetate Production
- **Felipe Martinez**, Alvaro Orjuela, Gerardo Rodriguez, Cesar A Sánchez Sr.
- **4:20** Paper 202c: Classification and Comparison of Dividing Wall Columns **Zewei Chen**, Rakesh Agrawal
- **4:45** Paper 202d: Transesterification in the Reactive Dividing Wall Column Energy Minimum Design and Operation *Laura-Selin Harding*, *Lisa Egger*, *Georg Fieg*
- **5:10** Paper 202e: Study on the Separation of Cyclohexane-Benzene Azeotrope via Extractive Distillation. I: Selection of Certain Deep Eutectic Solvents as Entrainers
- **Fang Bai**, Chao Hua, Ping Lu, Xu
- **5:35** Paper 202f: The Separation of Multi-Glycols with Divided-Wall Column *Yanyang Wu, Xinchuan Qu, Yuxian Yao*
- 5:59 Concluding Remarks

(203) Dust Explosions and Process Safety in Solids Processing

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 21 Chad Mashuga, Chair Ashok G. Dastidar, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- **3:30** Paper **203a:** Dust Particle Flow-Field Characterization Using High-Speed Digital In-Line Holography (DIH) During Minimum-Ignition Energy Testing
- Christian Schweizer, Ankit Saini, Daniel Guildenbecher, Chad Mashuga, Waruna Kulatilaka
- **3:48** Paper **203b**: Influence of Particle Density on Pre-Ignition Dust Cloud Dynamics in a Minimum Ignition Energy Testing Apparatus Using Digital In-Line Holography
- Ankit Saini, Christian Schweizer, Pranav Bagaria, Purvali Chaudhari, Waruna Kulatilaka, Chad Mashuga
- **4:06** Paper 203c: Effect of Particle Morphology on Dust Cloud Dynamics *FNU Shrey*, *Pranav Bagaria*, *Christian Schweizer*, *Chad Mashuga*
- **4:24** Paper 203d: Minimum Ignition Energy (MIE) prediction from QSPR using machine learning
- **Purvali Chaudhari**, Nilesh Ade, Lisa M. Perez, Stanley P. Kolis, Chad Mashuga
- **4:42** Paper 203e: The Characterization and Use of Limestone Rock Dusts in Coal Mines to Prevent Dust Explosions *Isaac Zlochower*
- **5:00** Paper 203f: Mitigation of Iron and Aluminum Dust Deflagrations Via Active Explosion Suppression in 1-m₃ Sphere Vessel
- Nicholas Reding, Mark B. Shiflett

(204) Effects of Confinement on Molecular Properties

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Rainbow Spring I/II

Liangliang Huang, Chair Liqun Zhang, Co-Chair

- **Sponsored by:** Thermodynamics and Transport Properties
- **3:30 Paper 204a:** Understanding the Effect of Radial Confinement on Phase Behavior of Surfactants
- **Yao Wu**, Yingzhen Ma, Bhuvnesh Bharti, William A. Shelton Jr.
- **3:43 Paper 204b:** Molecular Dynamic Simulation Study on the Air/Water-Alkanes Interface Systems
- Yi-lun Lee, Liqun Zhang
- **3:56 Paper 204c:** Confined Dynamics and Transport Properties of Organic Compounds
- **Siddharth Agrawal**, Michael P. Hoepfner

- **4:09** Paper 204d: Surface Confinement-Induced First Adsorbed Water Layer and Its Wettability Transition Under Compressive Lattice Strain
- **Guobing Zhou**, Liangliang Huang, Bradley Schoen, Zhen Yang
- **4:22** Paper 204e: Quantification of the Thermodynamic Effects Regarding Alkane Adsorption within ZSM-5 Using Advanced Sampling Grand Canonical Monte Carlo Simulations
- Christopher Rzepa, Daniel W. Siderius, Harold W. Hatch, Vincent Shen, Srinivas Rangarajan, Jeetain Mittal
- 4:35 Break
- **4:45** Paper 204f: A New Experimental Methodology for the Study of Hydrocarbon Phase Behavior Under Confinement

 Theodor Videnberg, Inês Graca, J. P.
- Theodor Videnberg, Inês Graça, J. P. Martin Trusler
- **4:58** Paper 204g: Study of Fluid Phase Equilibria of Triangle-Well Mixtures in Bulk and Under Confinement Using Grand Canonical Transition Matrix Monte Carlo *Tamaghna Chakraborti, Jhumpa*
- **5:11** Paper 204h: Programming Pore Uptake and Demixing of Surfactant Solutions in Spatially Confined Pores Yingzhen Ma, Yao Wu, Lilin He, Gernot Rother, William A. Shelton Jr., **Bhuvnesh Bharti**
- **5:24 Paper 204i:** Molecular Dynamics Simulations of Biomass-Modified Model Asphalt
- **Kolawole Sonibare**, Loukas Petridis, Liqun Zhang
- **5:37 Paper 204j:** Quantitative Modeling of Behavior of Water in Hydrophobic Confinement
- **Sumit Sharma**, Mohsen Ghasemi, Saeed Miri Ramsheh
- **5:50 Paper 204k:** On the Performance of Confined Deep Eutectic Solvents and lonic Liquids for Separations of Carbon Dioxide from Methane
- Yan Shen, Francisco R. Hung

(205) Electronic Structure Tuning in Catalysis

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Florida Ballroom C

Craig Plaisance, Chair Kostas Goulas, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30** Paper **205a**: Atomically Precise Gold Clusters with Modulated Ligand and Support Environment for Oxidation Catalysis
- **Nidhi Kapil**, Michael M. Nigra, Marc-Olivier Coppens
- **3:50 Paper 205b:** From Clusters to Single Atoms: Site Requirements for Carbon Monoxide Oxidation on Transition Metal and Metal Oxide Catalysts
- Zhuole Lu, Petar Lachkov, Thomas Kropp, Manos Mavrikakis, **Ya-Huei** (Cathy) Chin

- **4:10** Paper 205c: Electronic Structure Engineering in Heterogeneous Catalysis: From Simple Analytical to Machine Learnt Models of Chemisorption on Alloys *Suljo Linic*
- **4:50 Paper 205d:** Impact of Intrinsic Surface Strain on Electrocatalytic Processes
- Zhenhua Zeng, Lei Wang, Chao Wang, **Jeffrey Greeley**
- **5:10** Paper 205e: Hydrogen Evolution Activity and Water Oxidation Selectivity Tuning By Intermediate-Band Oxides
 Shu Hu
- **5:30** Paper 205f: Dynamic Modulation of Catalyst Electronic Structure to Enhance Reaction Rates
- **M. Alexander Ardagh**, Yan Wang, Omar A. Abdelrahman, Qi Zhang, C. Daniel Frisbie, Paul Dauenhauer

(206) Engineering Geologic Carbon Dioxide Storage Systems

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Challenger 41/42

Kanwal Mahajan, Chair Rameshwar D. Srivastava, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

- **3:30** Paper **206a**: Toward a Risk-Based Approach to Justify for Closure at Geologic Carbon Storage Sites
- **Robert Dilmore**, Diana H. Bacon, Grant Bromhal, Christopher F. Brown, Susan A. Carroll, Christine Doughty, Nicolas J. Huerta, Curtis M. Oldenburg, Rajesh Pawar, Xianjin Yang
- **3:51 Paper 206b:** Investigation of Mass Transfer and Sorption in CO₂/Brine/Rock Systems via *in-situ* FT-IR
- **Zhuofan Shi**, Sean Sanguinito, Angela Goodman, Theodore Tsotsis, Kristian Jessen
- **4:12 Paper 206c:** Thermodynamic Phase Behavior of ${\rm CO_2}$ Storage in Tight Formation
- Kaiqiang Zhang, Lirong Liu, Na Jia
- **4:33** Paper 206d: Regrid: A Python Toolbox for Reservoir Simulation Reproducibility, Comparison, and Multiphysics Code Interoperability
 Trevor Irons, Wei Jia, Brian McPherson
- **4:54** Paper **206e:** CO₂ Utilization for Enhanced Oil Recovery and Geologic Storage in Ohio
- **Rick Peterson**, Srikanta Mishra, Jared Hawkins, Manoj Valluri, Samin Raziperchikolaee, Ashwin Pasumarti, Isis Fukai, Andrew Duguid, Mark Moody
- **5:15** Paper 206f: Field Testing of Emerging Techniques for Active Management and Monitoring of Commercial CO₂ Storage
- **John A. Hamling**, Ryan J. Klapperich, Cesar Barajas-Olalde, Shaughn Burnison, Nicholas Bosshart

- **5:36 Paper 206g:** Modeling of the Formation of Carbon Dioxide Hydrate in Porous Media
- Tatsuya Fuji, Toru Sato, **Alan Junji Yamaguchi**, Hiroyuki Oyama, Takaomi Tobase

(207) Free Forum on Engineering Education: Junior and Senior Years II Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 23 Z. Otero Gephardt, Chair

Nastassja Lewinski, Co-Chair Sponsored by: Undergraduate Education

- **3:30 Paper 207a:** National Academies Transforming Separation Science Report: Chemical Engineering Separations Curricula
- **Joan F. Brennecke**, David S. Sholl
- **3:45** Paper 207b: Regional, Institutional, and Departmental Factors Associated with Gender Diversity Among Chemical and Electrical Engineering Graduates
- Laura Jarboe
- **4:00** Paper 207c: Implementing a Small-Scale Heat Transfer Radiative Experiment for Classroom Implementation
- Jacqueline Burgher Gartner
- **4:15** Paper 207d: Knowledge Laboratories: Approach to Facilitate Independent Inquiry and Experiential Learning for 2nd Year Students

 Pavan Inquiva, Mingrou Xie, Umang
- Pavan Inguva, Mingrou Xie, UmangV. Shah, Clemens Brechtelsbauer
- **4:30** Paper 207e: Improved Homework Effectiveness in a Problem-Solving Course
- Carl R. F. Lund
- **4:45** Paper 207f: Work in Progress: An Undergraduate "Introduction to Research Methods" Course for Honors Students
- Joseph H. Holles
- **5:00** Paper 207g: Participatory Design As a Tool to Develop Advanced Experiential Learning Projects for Chemical Engineering Students
- **Pavan Inguva**, Assen Batchvarov, Umang V. Shah, Clemens Brechtelsbauer

(208) Fundamentals of Catalysis II: C1 Chemistry

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom D Bryan R. Goldsmith, Chair Zhenxing Feng, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 208a: Adsorption and Activation of O₂ over Cu(I/II) Single-Site — *Feng Ryan Wang*

- **3:48 Paper 208b:** CO Oxidation By Pt Single Atoms and PtnO_x Clusters on Ceria
- Hui Wang, Jin-Xun Liu, Lawrence Allard, Sungsik Lee, Jilei Liu, Hang Li, Jianqiang Wang, Jun Wang, Se Oh, Wei Li, Maria Flytzani-Stephanopoulos, Meiqing Shen, **Bryan R. Goldsmith**, Ming Yang
- **4:06** Paper **208c**: Tuning Surface Properties of Titanium Dioxide for Carbon Monoxide Oxidation over Copper-Titanium Dioxide
- Guoqiang Cao, Nan Yi
- **4:24** Paper 208d: A Detailed Kinetics Study for Complete Methane Combustion over Ni/CexZr₁-XO₂ catalysts *Junjie Chen*, *Benjamin Carlson*, *Jae-Soon Choi*, *Zhenglong Li*, *Todd J. Toops*, *Eleni A. Kyriakidou*
- **4:42** Paper **208e**: An in Situ Formed Metastable Active Site Catalyzes the Formation of the Carboxyl Intermediate during the Water-Gas Shift Reaction *Nicholas Nelson*, *Janos Szanyi*
- **5:00** Paper **208f**: Bistability of the Fischer Tropsch Reaction over Promoted Co/MnO₂ Catalysts
- Norbert Kruse
- **5:18** Paper 208g: Cooperativity between Pd and AgO_x Phases on Ag(111) *Vikram Mehar*, *Ming-Hung Yu*, *Jason F. Weaver*
- **5:36** Paper 208h: The Challenge of CO Hydrogenation to Methanol: Fundamental Limitations Imposed By Linear Scaling Relations
- **Ahmed O. Elnabawy**, Pallavi Bothra, Julia Schumann, Jens K. Nørskov

(209) Fundamentals of Sustainability Science and Engineering

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Blue Spring I/II Bhavik R. Bakshi, Chair Heriberto Cabezas, Co-Chair

Sponsored by: Fundamentals

- **3:30** Paper 209a: Towards a Comprehensive Decision-Support Framework for Sustainable Manufacturing
- **Majid Moradi Aliabadi**, Yinlun Huang
- **3:55 Paper 209b:** Evaluating Dynamic Resilience of Intermittent and Uncontrollable Techno-Ecological Systems
- **Utkarsh Shah**, Bhavik R. Bakshi
- **4:20 Paper 209c:** A Multi-Layer Process Control Framework for Sustainability: Application to Biomass/Coal Co-Gasification System
- **Shuyun Li**, Gerardo J. Ruiz-Mercado, Fernando V. Lima
- **4:45** Paper 209d: Process Engineering Inspired Comparison of Sustainability and Resilience Specific Features of Natural and Human-Built Process Systems
- Bela Csukas, Monika Varga

- **5:10** Paper 209e: An Input-Output Framework to Assess the Importance of Insect Pollinators to US Industry Sectors: A Case Study of Apple Production
 Alex Jordan, Harland Patch,
 Christina Grozinger, Vikas Khanna
- **5:35** Paper **209f**: Rapid Estimation of Release Inventories and Evaluation: A U.S. Metal Coating Industry Case Study *Jose D. Hernandez-Betancur*, *Gerardo J. Ruiz-Mercado, Hugo Hernandez, Luz M. Ocampo-Carmona*

(210) Graduate Student Competition in Microbiointerface Research Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Celebration 9

Amy J. Karlsson, Chair

Elizabeth J. Stewart, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

- **3:43** Paper 210b: Heat Effects on Viability, Morphology, and Dispersal of Staphylococcus Epidermidis Biofilms
 Joanne Beckwith, J. Scott Van
- **3:56 Paper 210c:** Thermal Shock Dynamics on Biofilm Viability at Biomedical Interfaces

Epps, Michael J. Solomon

- Haydar Aljaafari, Eric Nuxoll
- **4:09 Paper 210d:** Structuring Microbial Biofilms with 3D Printing
- Reha Abbasi, James Wilking
- **4:22 Paper 210e:** The Role of Bacterial Chemotaxis in Improving Bioremediation Efficiency
- Xueying Zhao, Roseanne M. Ford
- **4:35 Paper 210f:** Antibacterial and Angiogenic Multifunctional Adhesives for the Treatment of Chronic Wounds
- Bahram Saleh, Thomas J. Webster
- **4:48** Paper 210g: Study of Collagen Tethered Antimicrobial Peptide Binding and Antimicrobial Activity
- **Ziqi Wei**, Lindsay D. Lozeau, Marsha W. Rolle. Terri A. Camesano
- **5:01** Paper **210h**: Fusogenic Liposomes Functionalized with Cell Penetrating Peptides for the Treatment of Bacterial Meningitis
- **Caterina Bartomeu Garcia**, Di Shi, Thomas Webster
- **5:14 Paper 210i:** Eradication of Bacterial Persister Cells By Targeting Membrane Potential
- **Sweta Roy**, Ali Adem Bahar, Huan Gu, Dacheng Ren
- **5:27 Paper 210j:** Nano-Tellurium (Te)-Titanium Synergetic Antibacterial Coatings for Biomedical Applications
- **David Medina**, Ada Vernet Crua, jose Miguel garcia Martin, Thomas J. Webster
- **5:40** Paper 210k: Mucoid Switch Enables a Growth Advantage to Pseudomonas Aeruginosain Interfacial Environments
- **Sricharani Balmuri**, Nicholas Waters, Tagbo H.R Niepa

(211) Green Chemistry and Engineering

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom U Christina Tang, Chair

Lindsay Soh, Co-Chair Clayton S Jeffryes, Co-Chair

Sponsored by: Sustainability Science and Engineering

- **3:30 Paper 211a:** Creation of a Chemical Synthesis Web Application Based upon a Chemical Reaction Ontology
- William M. Barrett, Sudhakar Takkellapati, Kidus Tadele, Michael A. Gonzalez
- **3:52** Paper 211b: A Comparison of Polarclean, Gamma-Valerolactone and Their Mixture As Bio-Derived Solvents for Polysulfone Membrane Fabrication *Xiaobo Dong*, *Halle Shannon*, *Caleb Parker*, *Isabel Escobar*
- **4:14** Paper 211c: Novel Application of Waste Concrete to Clean up the Air and Improve the Reliability of Civil Infrastructure
- **Alexander Orlov**, Shrish Patel, Erandi Ariyachandra, Sulapha Peethamparan
- **4:36 Paper 211d:** Direct FeCO₃ Reduction with H₂
- **Astrid Loder**, Susanne Lux, Matthaeus Siebenhofer
- **4:58** Paper 211e: Recovery of Metals from Cathode of Lithium-Ion Batteries: A Closed-Loop Approach Using Oxalate Chemistry
- **Ankit Verma**, Grant Johnson, Rajkumar Kore, David R. Corbin, Mark B. Shiflett
- **5:20 Paper 211f:** Direct Regeneration of Degraded Cathodes to Reduce Li-lon Battery Cost and Enhance Materials Sustainability
- **Zheng Chen**, Yang Shi
- **5:42** Paper 211g: Analysis of the Environmental Impact of the Pig Iron Production Process By the 12 Principles of Green Chemistry
- Andressa Tairine Evangelista, Fernando Luiz Pellegrini Pessoa, Ewerton Emmanuel da Silva Calixto

(212) How to Prepare Yourself for Management

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 18 Shweta Karwa, Chair Kanwar D Singh, Co-Chair

Sponsored by: Professional Development

- **3:30** Paper 212a: Workshop–Part 1 "I Followed the Recipe, Where Is My Cake?": Important Questions to Ask in Considering Transition to Management Salvador Aldrett
- **4:30 Paper 212b:** Workshop--Part 2: I Know the Why. Now What?
- Shweta Karwa

5:30 Paper 212c: General Discussion — *Shweta Karwa*

(213) In Honor of Ruth Baltus II (Invited Talks)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Barrel Spring I Jamie Hestekin, Chair Basavaraju Agasanapura, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30 Paper 213a:** Opportunities and Challenges for Hydrogen Production Using Membranes
- Jennifer Wilcox
- **3:52** Paper 213b: Functionalized and Responsive Membranes: An Overview *Dibakar Bhattacharyya*, Anthony Saad, Ashish Aher, Mohammad Saiful Islam, Hongyi Wan, Andrew Colburn
- **4:14** Paper 213c: Modeling of Gas Transport and Adsorption Considering Liquid Generation during the Removal of Mercury from Flue Gas
- Uwe Beuscher
- **4:36** Paper **213d:** Advanced Membrane Materials for Environmental Liquid Separations
- Mary Laura Lind
- **4:58 Paper 213e:** Interfacial Junctions Control Ion Transport through Charge Patterned Membranes
- William A. Phillip
- **5:20** Paper **213f**: My Career: Discs, Rods, Flexible and Deformable Particles, and Some Side Trips Along the Way *Ruth E. Baltus*

(214) In Honor of the 2018 R.H. Wilhelm Award Winner II (Invited Talks)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Florida Ballroom B

Stacey D. Finley, Chair David J. Klinke, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30** Paper 214a: Mechanistic Modeling of the (Bio)Conversion of (Bio) Macromolecules
- Linda J. Broadbelt
- **3:55 Paper 214b:** Cyclooctene-Facilitated Low Temperature Aerobic Oxidation of Ethylbenzene with Solubilized Au Clusters Catalysts *Harold H. Kung*
- **4:20** Paper **214c:** Stability of Supported Metal Catalyst in Aqueous Phase Reactions
- Brent H. Shanks, Jiajie Huo
- **4:45 Paper 214d:** Chemical Recycling the Answer to Plastic Waste?
- **Kevin M. Van Geem**, Guy B. Marin
- **5:10 Paper 214e:** A View of Cancer Immunology through a Reaction Engineering Lens
- David J. Klinke

5:35 Paper 214f: Exploring the Diversity of Complex Metabolic Networks

- Vassily Hatzimanikatis

(215) Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage -Electrocatalyst Development

Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom Q

Anirudh Balram, 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

3:30 Paper 215a: Scalable Production of Nanostructured Electrocatalysts for the e-Refinery

— J. Ruud van Ommen

3:51 Paper 215b: Enhancing Interfacial Contact for Advanced All Solid State Batteries with a Cathode-Supported Solid Electrolyte Membrane Framework — *Xinzhi Chen, DeLong Xie, Yuanzhi*

— **Xinzhi Chen**, DeLong Xie, Yuanzhi Zhu, Peichao Lian, Dedong He, Yi Mei, Haihui Wang

4:12 Paper 215c: Machine Learning of Carbon Electrodes for Electric Double Layer Capacitors

— **Musen Zhou**, Alejandro Gallegos, Kun Liu, Jianzhong Wu

4:33 Paper 215d: Applications of α-Nickel Hydroxide Catalyst for Electrochemical Water Splitting

— **Anirudh Balram**, Hanfei Zhang, Sunand Santhanagopalan

4:54 Paper 215e: Strongly Coupled 3D Ternary Fe₂O₃@Ni₂p/Ni(PO₃)₂ Hybrid for Enhanced Electrocatalytic Oxygen Evolution at Ultra-High Current Densities — *Xiaodi Cheng Sr.*

5:15 Paper **215f**: Single Iron Atoms Supported on MOF-Derived *N*-Doped Carbon for Robust Electrochemical CO₂ Reduction

- Tingting Wang

5:36 Paper 215g: Nickel Nanoparticles Embedded N-Doped Carbon Nanotubes As Biocompatible Electrocatalysis for CO₂ Conversion

— Zhongjian Li, Yang Hou**, Siyuan Xiu**, Gang Li

(216) Modeling and Analysis of Chemical Reactors II: The Impact of Dynamics on Reactor Design

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Plaza

International Ballroom F Sarah Feicht, Chair Justin A. Federici, Co-Chair Anthony G. Dixon, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 216a: Internal and External Diffusional Effects on the Selectivity of C₂ Products in Oxidative Coupling of Methane

— **Zhe Sun**, David West, Balakotaiah Vemuri

3:52 Paper 216b: Pattern Formation Insights from Computational Fluid Dynamics Modeling of Exothermic Shallow Packed Bed Reactors

— **Lei Chen**, Sreekanth Pannala, Robert Broekhuis, Pankaj S. Gautam, Tian Gu, David West, Balakotaiah Vemuri

4:14 Paper 216c: Experimental and Modeling Study of Passive NO_x Adsorbers: Pd-H-ZSM-5

- Michael Harold, Mugdha Ambast

4:36 Paper 216d: Parametric Sensitivity and Runaway in Fixed-Bed Reactors: Example of Methanol Selective Oxidation over Pt-Bi Catalysts

- Yang Xiao, Arvind Varma

4:58 Paper 216e: Ultimate Bounds on Reaction Selectivity for Batch Reactors — *Jeffrey A. Frumkin*, *Michael F. Doherty*

5:20 Paper **216f**: Bistability and pH Oscillations in the Urea-Urease Reaction in a Flow Reactor

— **František Muzika**, Ilgin Emel Karakoç, Lenka Schreiberova, Igor Schreiber

5:42 Paper **216g**: Modeling and Optimization of Industrial Ethylene Oxide Reactor for Deploying Real-Time Optimization Control Layer

— **Şahin Sarrafi**, Stepan Spatenka, Mayank Patel, Sinan Üçyiğitler, Yaşar S. Kabak, Ahmet K. Avci, Yaman Arkun, Fikret Inal

(217) NSF Workshop II: Proposal Writing and Discussions with Program Managers

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 29/30 Ram B. Gupta, Chair Richard Dickinson, Co-Chair

Sponsored by: Career Guidance Committee Liaison

3:30 Paper 217a: Proposal Writing Tutorial

- Dimitrios V. Papavassiliou

4:30 Paper 217b: Interactive Breakout Panels

— **Richard Dickinson**, Carole Read, Steven Peretti, Carl Rockne, William Olbricht

(218) Numerical Analyses of Mixing Processes in Bioreactors

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 32 Justin Walker, Chair Eric E. Janz, Co-Chair

Sponsored by: North American Mixing Forum

3:30 Paper 218a: Towards an Understanding of Fluid History in a Turbulent Mixing Tank Using Large Eddy Simulation Model

— **Matthew H. Flamm**, Katherine Raudenbush, Eric Sirota, Aaron Cote

3:51 Paper 218b: CFD Modelling and Matlab Analysis to Asses Mixing Performance in Custom Vessel Configurations in the Biopharmaceutical Industry

- Jamie McCarry

4:12 Paper **218c**: Spiroid Design Optimization in a Rotating Continuous Bioreactor for Enhanced Oxygen Mass Transfer

— **Rithvija Avvari**, Paul W. Todd, Thomas R. Hanley

4:33 Paper 218d: Effect of Gas Sparge Type on Oxygen Mass Transfer in an Agitated Vessel (comparing CFD versus Experimental Modeling Techniques)

— John A. Thomas, Richard Kehn

4:54 Paper 218e: Multiphase Reacting Flow Simulations and Optimization of Commercial-Scale Aerobic Bioreactors — *Hariswaran Sitaraman*, *Mohammad J. Rahimi, James J. Lischeske, Jonathan J. Stickel*

5:15 Paper 218f: Modeling Mixing in Aerated Systems: Mass Transport and Flooding

- Christopher Tyler, John A. Thomas

5:36 Paper 218g: CFD Simulation of Gas-Liquid Flow in Stirred Tanks: Effect of Drag Models

— **Xiaoping Guan**, Xinju Li, Ning Yang, Mingyan Liu Sr.

(219) Panel Discussion: Advice and Mentorship from Female Leaders in Innovation and Entrepreneurship (Invited Talks)

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom N

Whitney L. Stoppel, Chair Anita Shukla, Co-Chair Julie N. Renner, Co-Chair

Sponsored by: Women in Chemical Engineering Committee (WIC)

(220) Particle Breakage and Comminution Processes

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 20 Ecevit Bilgili, Chair Sarang Oka, Co-Chair

Sponsored by: Particle Production and Characterization

3:30 Paper 220a: Are Crosslinked Polystyrene Beads As Effective As Zirconia Beads to Produce Drug Nanoparticles Via Wet Stirred Media Milling?

— Nathaniel Parker, Mahbubur Rahman, **Ecevit Bilgili** **3:51 Paper 220b:** Understanding the Flow of Calcium Carbonate in Stirred Media Mills

— **Sophie Rimmer**, Andrew Ingram, Richard Tamblyn, Federico Alberini

4:12 Paper 220c: Time and Energy Dependent Properties of Stirred Wet Milled Alumina-Doped Titanium Dioxide, a Discretely Heterogeneous System — *David Austin, David Harbottle, Timothy N. Hunter, Ali Hassanpour*

4:33 Paper 220d: Influence of Particle Properties and Volume Fraction on the Velocity of Particle in Grinding Zone of Jet Mill: Particle Tracking Velocimetry (PTV) and CFD-Dpm Model

— **Mahesh Dhakate**, Devang V. Khakhar, Jyeshtharaj B. Joshi

4:54 Paper 220e: From Particle to Process Predicting Breakage of Structured Particles

- Kerry Johanson

5:15 Paper 220f: Milling Studies in an Impact Crusher I: Kinetics Modelling Based on Population Balance Modelling — Ngonidzashe Chimwani, Murray M Bwalya

5:36 Paper 220g: A Mechanistic Collision Model for Particle Breakage in Agitated Crystallization Experiments — *Rory Tyrrell, René R. E. Steendam, P.J. Frawley*

(221) Poster Session: Fluid Mechanics

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom M Simon Rogers, Co-Chair Joseph R. Samaniuk, Co-Chair

Sponsored by: Fluid Mechanics

Paper 221a: Rheological Characterization of Dynamic Remodeling of the Pericellular Region By Human Mesenchymal Stem Cell-Secreted Enzymes in Synthetic Hydrogel Scaffolds

Kelly M. Schultz, Maryam DaviranPaper 221b: Geostatistical Inversion

Technique for Thin Sandstone Modeling

— Muneera Al-Awadhi, Adel

Elsharkawy

Paper 221c: Simulations of Reactive Transport with the Openfoam Toolkit — Anthony J.C. Ladd, Vitaliy Starchenko

Paper 221d: Diffusiophoretic Spreading Under Localized, Transient Solute Gradients: From Trapping to Super-Diffusion — Henry C. W. Chu, Stephen Garoff, Robert D. Tilton, Aditya S. Khair

Paper 221e: Theory and Experiments of Measuring Microrheology Via Dynamic Magnetic Susceptibility

— Mingyang Tan, Partha Paul, Pallavi Dhagat, **Travis W. Walker** Paper 221f: Flow Analysis of Human Blood Using a Compact-Sized Falling Needle Rheometer (FNR) and Correlation Using Modified Constitution Equation Based on Herschel-Bulkley Model

— **Yusuke Negi**, Takafumi Yabuta, Hideki Yamamoto Sr.

Paper 221g: Additive Manufacturing with Soft Tpu: Thermal Properties for Printability and Adhesion Strength in Multimaterial Flexible Joints

— Şebnem Özbek, Conor G. Harris, Whytneigh R. Duffie, Willie E. "Skip" Rochefort, Travis W. Walker

Paper 221h: Capsule Dynamics in a Microfluidic Cross-Junction — Pompon Mputu Udipabu, Panagiotis Dimitrakopoulos

Paper 221i: An Inhomogeneous, Nonequilibrium Thermodynamics Approach to Modeling Blood Rheology — Jeffrey S. Horner, Soham Jariwala, Yu-Jiun Lin, Antony N. Beris, Norman J. Waaner

Paper 221j: Particle Migration in Confined Channel

— Atul M. Bhagat, Partha S. Goswami

Paper 221k: Electrohydrodynamics of Drops in Randomly Fluctuating Electric Fields

— **Rajarshi Sengupta**, Lynn M. Walker, Aditya S. Khair

Paper 221I: Calibration of Chromatographic Effects in Capillary Flow — Katrina J. Donovan, James Stasiak, Willie E. "Skip" Rochefort

Paper 221m: Investigation of Two-Phase Flow Characteristics in a Fractal-Branching Microchannel

— **Sahar Hajizeinalibioki**, Daniel Sebastia-Saez, Oleksiy V. Klymenko, Harvey Arellano-Garcia

Paper 221n: Effects of Internal Structures on Capsule Lateral Migration — Abdollah Koolivand, Panagiotis Dimitrakopoulos

Paper 221o: Molecular &
Macromolecular Engineering of Foams
— Vivek Sharma, Chenxian Xu, Carina
Martinez, Chrystian Ochoa

Paper 221p: Free Surface Flows and Extensional Rheology of Polymer Solutions

- Jelena Dinic, Vivek Sharma

Paper 221q: Influence of Film Size on Drainage of Foam Films

— **Maulik Shah**, Volkert van Steijn, Chris R. Kleijn, Michiel Kreutzer

Paper 221r: Rheological Characterization of Dynamic Remodeling of the Pericellular Region By Human Mesenchymal Stem Cell-Secreted Enzymes in Well-Defined Synthetic Hydrogel

— **Maryam Daviran**, sarah M. Longwill, Jonah F. Casella, Kelly M. Schultz Paper 221s: Interplay between Swimming Speeds, Motor Torques and Filament Numbers in Multi-Flagellated Cells

- Kathy Rhee, Pushkar Lele

Paper 221t: Method of Controlling the Shape of Cube-like Hematite Particles and Influence of Externalmagnetic Field on the Aggregate Structures

— **Kazuki Yatabe**, Keita Oda, Akira Satoh, Muneo Futamura

Paper 221u: Accuracy Evaluation of Finite Volume Method based Direct Numerical Simulation for Solving Highly Turbulent Flows

— **Shashank S. Tiwari**, Zhizhong Ding, Ashwin W. Patwardhan, K. Nandakumar, J. B. Joshi

(222) Precision Medicine, Big Data, and Chemical Engineering

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Celebration 12/13

Sammy S. Datwani, Chair Lydia M. Contreras, Co-Chair

Sponsored by: Chemical Engineers in Medicine

3:30 Paper 222a: Tracking Epitranscriptomics Modifications to Understand Early Health Effects of Oxidative-Prone Air

— Juan Camilo Gonzalez, **Lydia M. Contreras**

3:51 Paper 222b: Tunneling Spectroscopy for Sequence and Structural Label Determination in Single DNA and RNA Molecules

— **Lee Korshoj**, Gary Abel Jr., Anushree Chatterjee, Prashant Nagpal

4:12 Paper 222c: Profiling Cell-Type-Specific Epigenomic Changes Associated with BRCA, Mutation in Breast Tissues Using a Low-Input Microfluidic Technology

— **Yuan-Pang Hsieh**, Lynette Naler, Xiaowen Zhang, Travis Murphy, Rong Li, Chang Lu

4:33 Paper 222d: A Metabolomics Approach to Predict Chemotherapy-Induced Peripheral Neuropathy

— **Parul Verma**, Jamie Renbarger, Jodi Skiles, Bruce Cooper, Doraiswami Ramkrishna

4:54 Paper 222e: An Exposome Connectivity Paradigm for the Mechanistic Assessment of the Effects of Prenatal and Early-Life Exposure to Metals on Neurodevelopment

— **Dimosthenis Sarigiannis**, Nafsika Papaioannou, Maria Fafouti, Michael Dickinson, Aikaterini Gabriel, Spyros Karakitsios

5:15 Paper 222f: A Systems Approach to Understanding Drug Response in a Heterogeneous Tumor-Cell Population

— James Park, Adrian Lopez Garcia de Lomana, Parvi Hothi, Charles Cobbs, Sui Huang, Nitin Baliga **5:36** Paper 222g: Quantitative Label-Free Interference-Based Phenotyping of Cancer Cells for Liquid Biopsy Applications

— **Jose C. Contreras-Naranjo**, Arul Jayaraman, Victor M. Ugaz

(223) PSA/TSA

Exchange

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Manatee Spring I Roger D. Whitley, Chair

Reza Haghpanah, Co-Chair

Sponsored by: Adsorption and Ion

3:30 Welcoming Remarks

3:35 Paper 223a: Water Vapour Capture on MIL-125(Ti)_NH₂ By (P)TSA Process

— Márcia Silva, Ana M. Ribeiro, Cláudia G. Silva, Guler Narin, Idelfonso Nogueira, U-Hwang Lee, Joaquim L. Faria, Jong-San Chang, Alirio Rodrigues, **Alexandre Ferreira**

3:55 Paper 223b: Dynamic Behavior of Pressure Swing Adsorption Process for Nitrous Oxide Recovery from the Off-Gas of Adipic Acid Production

— **Dooyong Park**, JeongHoon Kim, Hyungwoong Ahn, Chang-Ha Lee

4:15 Paper **223c**: Equilibrium Theory Analysis of Equalization Tanks in a PSA Process

— **Behnam Fakhari Kisomi**, Armin D. Ebner, James A. Ritter

4:35 Paper 223d: An Equilibrium-Based Shortcut Temperature Swing Adsorption (TSA) Model for Screening Adsorbents for Heavy Component Recovery

— **Abdulmalik Ajenifuja**, Lisa Joss, Megan Jobson

4:55 Paper 223e: Sub-Ambient Pressure Swing Adsorption Enabling High Capacity CO, Capture

— Stephen J.A. DeWitt, Ryan Lively

5:15 Paper 223f: Experimental Validation of PSA Optimization Techniques

— Libardo Estupinan-Perez, Partha Sarkar, **Arvind Rajendran**

5:35 Paper 223g: Evaluation of Structured Adsorbents for Carbon Capture Applications

— Shreenath Krishnamurthy, Richard Blom, Carlos Grande, Anna Lind, Robert De Boer, Soraya Sluijter

(224) Reaction Chemistry and Engineering II: Catalysis and Process Intensification

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom E Kaiwalya Sabnis, Chair Josh Allen, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 224a: Active Sites and Mechanisms for Vapor-Phase Decomposition of Formic Acid on Pt Catalysts
— Saurabh Bhandari, Srinivas Rangarajan, Christos T. Maravelias, James A. Dumesic, Manos Mavrikakis

3:50 Paper 224b: Direct
Decomposition of NO Using Specialized
Metal Oxides in a Novel Chemical
Looping Reactor System
— Deven Baser, Peter Sandvik, Zhuo

4:10 Paper **224c**: The Effect of Physiochemical Properties of Copper Oxide Sorbents on the Chemisorptive Removal of Sulfur

Cheng, Liang-Shih Fan

— **Sara Azzam**, Faisal Alshafei, Tirso Lopez-Ausens, Richa Ghosh, Brian KO, Dante Simonetti

4:30 Paper 224d: Chemical Reduction in Gas-Liquid Plasma Reactors

— Robert Wandell, Radha Krishna Murthy Bulusu, Rony Gonzales, Bruce R. Locke

4:50 Paper **224e:** Kinetic Studies of Quaternary Ammonium Salt Degradation for Process Intensification Purposes — *Roel Kleijwegt, Wyatt Winkenwerder, John van der Schaaf*

5:10 Paper 224f: Enhanced NO, CO and C_3H_6 Conversions on Precious Group Metal Catalysts: Impact of Oxygen Storage Material and Catalyst Architecture

— **Zhiyu Zhou**, Michael Harold, Dan Luss

5:30 Paper 224g: Esterification of Dilute Aqueous Carboxylic Acids with Metallosurfactant Type Catalysts — *Andreas Toth, Silke Schnedl,*

Susanne Lux, Daniela Painer, Matthaeus Siebenhofer

(225) Recent Advances in Molecular Simulation Methods I

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Rock Spring I/II Harish Vashisth, Chair Andrew White, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

3:30 Paper 225a: Time-Independent Free Energy Surfaces from Time-Dependent Biased Simulations Via Thermodynamic Integration

— Veselina Marinova, Matteo

— **veseiina marinova**, Matted Salvalaglio

3:45 Paper 225b: Mapping Saddles and Minima on Free Energy Surfaces Using Multiple Climbing Strings

— Gourge Shrivestory Fric Vanden-

— **Gourav Shrivastav**, Eric Vanden-Eijnden, Cameron F. Abrams

4:00 Paper 225c: The Overdamped Transmission Coefficient: Recovering the True Mean First Passage Time from an Inaccurate Reaction Coordinate

— **Ryan Yappert**, Baron Peters, Kartik Kamat

- **4:15** Paper **225d**: Collective Mode Brownian Dynamics: A Method for Fast Relaxation of Statistical Ensembles *Kevin Silmore*, *James Swan*
- **4:30** Paper 225e: A New High-Throughput Computational Method to Generate Energy Profile of Integral Membrane Protein-Protein Association

 Nandhini Rajagopal, Shikha Nangia
- **4:45** Paper **225**f: Development of a New Coarse-Grained Model Capturing Hydrogen Bonding Effects in Polysaccharides
- **Zijie Wu**, Daniel J. Beltran-Villegas, Daniel Intriago, Arthi Jayaraman
- **5:00** Paper 225g: Implementation of Quantum Mechanics/Coarse-Grained Molecular Mechanics (QM/CG-MM)
- **Alexander V. Mironenko**, Gregory A. Voth
- **5:15** Paper 225h: An Alternative Model for Simulating Water between Two Phosphorylcholine Self-Assembled Monolayer Surfaces
- **Nan Xu**, Jianxiang Huang, Matthew T Bernards, Tao Xia, Yao Shi, Yi He
- **5:30** Paper **225i**: Van Hove Correlations in Aqueous Systems: Insights from Molecular Simulation — *Matt Thompson*, *Ray Matsumoto*,

Peter T. Cummings

- **5:45** Paper **225**j: Quantification of DNA Hybridization Thermodynamics at the Atomistic Level
- **Gul H. Zerze**, Frank H. Stillinger, Pablo G. Debenedetti

(226) Redox Flow Batteries for Energy Storage

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 28 Burcu Gurkan, Chair

Sponsored by: Transport and Energy Processes

- **3:30 Paper 226a:** Probing the Mechanisms of Aqueous-Phase V²⁺/V³⁺ and Ce³⁺/Ce⁴⁺ Redox Reactions for Redox Flow Batteries
- **Nirala Singh**, Harsh Agarwal, Cailin Buchanan, Jacob Florian, Eunbyeol Ko, Bryan R. Goldsmith
- **4:00** Paper 226b: Design and Optimization of a Vanadium Redox Flow Battery for Load-Following Applications Sai Pushpitha Vudata, Debangsu Bhattacharyya, Richard Turton
- **4:25** Paper 226c: Scalable Faradaic Electrodes for Enhanced Charge Transfer in Redox Flow Batteries

 Robert Emmett, Mark E. Roberts
- **4:50 Paper 226d:** Flexible Ceramic Membranes for High Performance Redox Flow Batteries
- Greg Newbloom
- **5:15** Paper 226e: Fluorenone Based Anolyte for an Aqueous Organic Redox-Flow Battery
- **Jaime Rodriguez Jr.**, Claire Niemet, Lilo Pozzo

(227) Renewable Fuels Production from Captured CO, and Hydrogen

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Regency Ballroom P

Maxim Lyubovsky, Chair

Sponsored by: Synthetic & Renewable Fuels

- **3:30 Paper 227a:** Department of Energy's Carbon Capture and Utilization R&D Portfolio and Applications to Renewable and Synthetic Fuels
- Lynn Brickett, Amishi Kumar
- **4:00 Paper 227b:** Capturing CO₂ from the Atmosphere
- Todd Wilke
- **4:30** Paper 227c: Sustainable and Renewable Carbon and Nitrogen Cycles for Fuel and Crop Production
- Daniel G. Nocera
- **5:00 Paper 227d:** Carbon Capture and Conversion: The Methanol EconomyR
- Surya Prakash
- **5:30** Paper **227e**: Technical and Economic Feasibility of Electron-Driven CO₂ Reduction
- **Joshua A. Schaidle**, Ling Tao, Gary Grim, Zhe Huang

(228) Session in Honor of Prof. Atsushi Tsutsumi's Accomplishments

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 19 Ray Cocco, Chair Mikio Sakai, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

- **3:30 Paper 228a:** Chemical Looping Technology a Particle Technology Perspective
- L.-S Fan
- **3:50** Paper **228b**: Mass Production of Well Aligned Carbon Nanotubes and Carbon-Silicon Based Anode Materials By Fluidized Bed
- Fei Wei
- **4:10** Paper 228c: Novel Fluidized Bed Reactors for Biomass Thermochemical Conversion
- **Xiaotao Bi**, Jim C. Lim, Naoko Ellis, John R. Grace
- **4:30 Paper 228d:** Gasification of Biomass Particles: Biochar Production, Particulate Emission, and Process
- Ye Shen, Zhiyi Yao, Liping Wei, **Chi-Hwa Wana**
- **4:50 Paper 228e:** Development of a Triple-Bed Combined Circulating Fluidized Bed
- **Chihiro Fushimi**, Guoqing Guan
- **5:10** Paper 228f: Green Energy Innovation for Sustainable Society:Exergy Recuperation Technology *Atsushi Tsutsumi*

(229) Sustainable and Green Product Design

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Bayhill 17 Sitaraman Krishnan, Chair Mu Wang, Co-Chair Kishori T. Deshpande, Co-Chair

Sponsored by: Product Design

- 3:30 Welcoming Remarks
- **3:33** Paper **229a**: A Novel Multiscale Model Approach to Describe Products Formation during the Cultivation of *Haematococcus Pluvialis* Under Different Environmental Conditions *Alessandro Usai*, *Jon Pittman*,
- Constantinos Theodoropoulos

 3:51 Paper 229b: Optimization and
- Scale-up of Biodiesel Production
 Using Lipase Immobilized on Magnetic
 Nanoparticles
- **Imran Quasem**, Aydin K. Sunol, George Philippidis
- **4:09** Paper 229c: Process Design and Economic Analysis of the Production of Sucrose Esters Using a Solvent-Free Transesterification
- Maria F. Gutierrez, Alvaro Orjuela
- **4:27 Paper 229d:** The Dilemma of Formic Acid Stabilization: Key Influences of Stabilizers on the Esterification Reaction
- **Teresa Kaiser**, Mahsa Nozari, Andreas Jupke
- **4:45** Paper 229e: Thermodynamic Modeling of Kraft Black Liquor Solutions with the Electrolyte NRTL Model
- **Toni Kirkes**, Chau-Chyun Chen
- **5:03** Paper 229f: An Integrated Methodology for the Design of Optimal Solvent-Based Adhesive Products with Low Toxicity
- **Suela Jonuzaj**, Jingyue Cui, Claire S. Adiiman
- **5:21** Paper **229**g: A Novel Microporous Graphite Bipolar Plate Design for Effective Water Management in PEM Fuel Cells
- **Aswin Prathap Pitchiya**, Sitaraman Krishnan
- **5:39 Paper 229h:** Energy-Saving Self-Entrained Heterogeneous Azeotropic Distillation for Separating Immiscible Systems
- Ming Xia

(230) Thermodynamic and Transport Properties Under Pressure II Monday, Nov 11, 3:30 PM

Hyatt Regency Orlando, Plaza International Ballroom K Erdogan Kiran, Chair Sabine Enders, Co-Chair

Sponsored by: High Pressure

- **3:30 Paper 230a:** Jet Dynamics in Supercritical Fluid Flow
- **Hilary T. Fabich**, Mark S. Conradi, Stephen A. Altobelli, Dean O. Kuethe, Eiichi Fukushima

- **3:54** Paper **230b**: Supercritical Hydrothermal Synthesis Solvent Effect on Kinetics, Reaction Equilibrium and Solubility in Supercritical Water *Tadafumi Adschiri, Takaaki Tomai, Akira Yoko, Gimyeong Seong*
- **4:18** Paper 230c: High Pressure Viscosity of Poly(alpha olefin)s *Katrina Avery, Erdogan Kiran, James Dickmann, Mark Devlin*
- **4:42 Paper 230d:** Effect of CO₂ Pressure on the Viscosity of 1-Alkyl-1-Methylpyrrolidinium Bis(trifluoromethylsulfonyl)lmide lonic Liquids
- Ana R. C. Morais, Donna L. Baek, Robert V. Fox, Mark B. Shiflett, Aaron M. Scurto
- **5:06** Paper 230e: New Insight in the NaCI-H₂O Phase Diagram Under Pressure and Temperature

 Thomas Voisin, Arnaud Erriquible,
- **5:30 Paper 230f:** Hydrates-Based Seawater Desalination: A Comparative Study with Conventional Desalination

Cyril Aymonier

Processes

— Muhammad Khan, Sheraz Bashir, Cornelis Peters, Hongfei Xu, Carolyn

(231) Thermodynamics of Biomolecular Folding and Assembly

Monday, Nov 11, 3:30 PM Hyatt Regency Orlando, Silver Spring I/II Gul H. Zerze, Chair Aviel Chaimovich, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **3:30** Paper 231a: Protein-Solvent Attractive Interactions Dominate the Inverse Temperature of Polypeptide Hydration Free Energies
- Dheeraj Tomar, Michael Paulaitis, Lawrence R. Pratt, **Dilip Asthagiri**
- **3:45** Paper 231b: Thermodynamics of Protein Folding Near the Low-Temperature Liquid-Liquid Transition in Water: A Case Study with the Trp-Cage Miniprotein
- **Daniel J. Kozuch**, Frank H. Stillinger, Pablo G. Debenedetti
- **4:00** Paper 231c: Molecular Insights into Protein Liquid-Liquid Phase Separation from Simulation and Experiment
- **Gregory L. Dignon**, Gul H. Zerze, Anastasia C. Murthy, Alexander E. Conicella, Nicolas Fawzi, Jeetain Mittal
- 4:15 Paper 231d: Dense Liquid
 Condensates Host the Nucleation of
 Tumor Suppressor p₅₃ Fibrils
 Mohammad Safari, Anatoly
 Kolomeisky, Jacinta C. Conrad, Peter
 Vekilov

- **4:30** Paper 231e: Molecular Insights into the Surface Catalyzed Secondary Nucleation of Amyloid-β40 (Aβ40) By the Peptide Fragment Aβ16-22
- Yiming Wang, Samuel J. Bunce, Katie L. Stewart, Alison E. Ashcroft, Sheena E. Radford, Andrew J. Wilson, Carol K. Hall
- **4:45 Paper 231f:** Amyloid Fibrillization Mystery: Is Backtracking Real?
- **Yuechuan Xu**, Nicholas P. Schafer, Peter G. Vekilov, Peter G. Wolynes
- **5:00 Paper 231g:** Computational Modeling and Simulation Studies of Ligand Binding Problems
- Asuka A. Orr, Arul Jayaraman, Michael Manson, Stephen Safe, Dimitrios Morikis, Chrysoula Kokotidou, Anna Mitraki, Timothy D. Phillips, Phanourios Tamamis
- **5:15** Paper 231h: Coupled Computational/Experimental Approach to the Thermodynamics of Biomolecular Interaction
- **Erik Laurini**, Domenico Marson, Suzana Aulic, Andrea Mio, Maurizio Fermeglia, Sabrina Pricl
- **5:30** Paper 231i: Long Time-Scale Atomistic Simulations of HIV-1 TAR RNA

 Lev Levintov, Harish Vashisth

(232) Undergraduate Research Presentations - Materials and Biotechnology

Monday, Nov 11, 12:30 PM Hyatt Regency Orlando, Bayhill 31 Cory Thomas, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

(233) Tutorial on Nuclear Chemical Engineering Focusing on Nuclear Fuel Cycle (Invited Talks)

Monday, Nov 11, 4:15 PM Hyatt Regency Orlando, Discovery 43 Michael F. Simpson, Chair Supathorn Phongikaroon, Co-Chair

Sponsored by: Nuclear Engineering Division

- **4:15 Paper 233a:** Overview of Nuclear Fuel Cycle
- L. Larry Hamm
- **4:36** Paper 233b: Modeling and Simulation of Nuclear Fuel Processes *Valmor F. de Almeida*
- **4:57** Paper 233c: Aqueous Nuclear Fuel Reprocessing Processes *Anthony P. Gouge*
- **5:18** Paper 233d: Electrochemical and Molten Salt Applications as Non-Aqueous Reprocessing Technologies *Michael F. Simpson*
- **5:39 Paper 233e:** Isotope Separation Methods
- Maximilian B. Gorensek

(234) Engineers Can Do Anything: Explore Your Passions and Catalyze Your Potential to Create Your Unicorn Career

Monday, Nov 11, 4:45 PM Hyatt Regency Orlando, Orlando Ballroom L April Grasso, Chair

Sponsored by: Publication Committee

- **4:45** Paper 234a: Engineers Can Do Anything: Explore Your Passions and Catalyze Your Potential to Create Your Unicorn Career
- Alaina Levine

(235) MAC Eminent Engineers Awards Ceremony

Monday, Nov 11, 5:30 PM Hyatt Regency Orlando, Regency Ballroom O

Sipho C. Ndlela, Chair Kazeem Olanrewaju, Co-Chair

Sponsored by: Minority Affairs Committee (MAC)

(236) D.I.C. Wang Award Lecture Monday, Nov 11, 6:00 PM

Hyatt Regency Orlando, Regency Ballroom V

Sponsored by: Awards Committee

6:00 Paper 236a: From Artificial Cofactors to Synthetic Arrays: Teaching Old Enzymes New Tricks

- Douglas S. Clark

(237) Pharmaceutical Discovery, Development, and Manufacturing Forum Awards Ceremony

Monday, Nov 11, 6:30 PM Hyatt Regency Orlando, Regency Ballroom U

Mary T. am Ende, Chair Shujauddin M. Changi, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

(238) Ammonia Synthesis: Intrinsically Carbon-Free Production

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

8:00 Introductory Remarks

8:03 Paper 238a: Solid Oxide Technology for Ammonia Production and Use

- John Bøgild Hansen
- **8:26** Paper 238b: Demonstration and Optimization of Green Ammonia Production Operation Responding to Fluctuating Hydrogen Production from Renewable Energy
- **Yasushi Fujimura**, Mototaka Kai, Takayoshi Fujimoto, Sho Fujimoto, Ryousuke Atsumi, Masayasu Nishi, Takehisa Mochizuki, Tetsuya Nanba

- **8:49 Paper 302a:** Technoeconomic Requirements for Sustainable Ammonia Production
- Nico Pinkowski, Brian A. Rohr, Joshua M. McEnaney, Jay Schwalbe, Michael Statt
- **9:12** Paper 238d: Coupling Integral Molten Salt Reactor to Ammonia Production Via Hybrid Sulfur (Hy-S) Process
 John Kutsch
- **9:35 Paper 238e:** Starfire Energy's 10 Kg/Day Rapid Ramp NH₃ System Development
- **Joseph Beach**, Jonathan Kintner, Adam Welch

(239) Advances in Bioseparations Tuesday, Nov 12, 8:00 AM

Hyatt Regency Orlando, Barrel Spring II Sutapa Barua, Chair Ketki Behere, Co-Chair

Sponsored by: Bio Separations

- **8:00 Paper 239a:** Lab-on-a-Chip Device for Shear Enhanced Purification of Macro Biomolecules
- **Pedro Moura**, Yu Hsuan Cheng, Zhenglong Li, Sagnik Basuray
- **8:20 Paper 239b:** Heme Extraction and Separation for the Preparation of Apphemoglobin
- Ivan Pires, **Donald Belcher**, Richard Hickey, Colbert Miller, Abraham Badu-Tawiah, Jin Hyen Baek, Paul Buehler, Andre Palmer
- **8:40 Paper 239c:** Separating Early Stage Amyloid Aggregates Using Microchannel Electrophoresis
- **Xavier Redmon**, Christa N. Hestekin, Melissa Moss, S. Zeb Vance
- **9:00 Paper 239d:** Characterization of Protein-Polymer Conjugates Using Aqueous Two-Phase Systems
- **Dylan Lewis**, Shelley L. Anna, Alan Russell
- **9:20** Paper 239e: Novel Enzymes and Separations in Biotechnology-Identifying a Process Tailored Extraction System-
- Maximilian Wessner, Gerhard Schembecker, Christoph Brandenbusch
- **9:40** Paper 239f: Optimization Opportunities of Virus Purification in Different Modes of Aqueous Two-Phase System
- **Pratik U. Joshi**, Michael Schroeder, Bianca Jones, Stephanie Kroger, Seth Kriz, Matthew Weiss, Glendy Escalante-Corbin, Silviya Petrova Zustiak, Caryn L. Heldt
- **10:00 Paper 239g:** Using Droplet-Based Millifluidic Platform to Separate Biomolecules in Aqueous Two-Phase Systems
- Yanxin Li, Shelley L. Anna

(240) Advances in Large Molecule Processes

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Celebration 7
Michael L. Hoffman, Chair
Dominique Hebrault, Co-Chair
Pouria Motevalian, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **8:00 Paper 240a:** Engineering Quality and Manufacturability of a Trivalent Protein Subunit Vaccine
- **Neil C. Dalvie**, Joseph R. Brady, Mary Kate Tracey, Laura Crowell, D. Lee Kristensen, Kerry Routenberg Love, J. Christopher Love
- **8:21** Paper 240b: Design of Experiments Reveals Critical Parameters for Bulk Freeze-Thaw of Lactate Dehydrogenase
- **Bruna Minatovicz**, Sameera Sansare, Robin Bogner, Bodhisattwa Chaudhuri
- **8:42** Paper 240c: Multimodal Membrane Adsorbers for Clearance of Minute Virus of Mice
- **Tanmoy Patra**, Shu-Ting Chen, Namila Khereid, S. Ranil Wickramasinghe, Xianghong Qian
- **9:03 Paper 240d:** Advances in Spray Freeze-Drying for Uniform Spherical Bulk Intermediate Product
- **Howard Stamato**, Bernhard Luy
- 9:24 Paper 240e: Controversial Influence of Gravitational Force on the Crystallisation of Lysozyme — Huaiyu Yang, Vikram Karde, Jerry
- **Huaiyu Yang**, Vikram Karde**, Jerr Y. Y. Heng**
- 9:45 Paper 240f: Application of CFD Modeling for the Development and Transfer of Mixing and Compounding Processes with Single Use Equipment Mario Hirth, Kushal Sinha, Nandkishor K. Nere, Martin Bultmann
- **10:06 Paper 240g:** Bio-Separation Via Selective Protein Crystallisation Facilitated By Porous Silica Templates: A Case Study Using Mesoporous Nanoparticles in Lysozyme-Thaumatin Mixture
- **Xiaoyu Li**, Wenqian Chen, Jerry Y. Y. Hena

(241) Advances in Life Cycle Optimization for Process Development

Tuesday, Nov 12, 8:00 AM

Hyatt Regency Orlando, Blue Spring I/II Debalina Sengupta, Chair Gonzalo Guillén-Gosálbez, Co-Chair

Sponsored by: Process Development

- **8:00** Paper 241a: A Multi-Objective Optimization Model to Plan City-Scale Water Systems with Economic and Environmental Objectives: A Case Study in Santiago, Chile
- **Javiera Riffo**, Daniela Gormaz, Ludovic Montastruc, Felipe Díaz

- **8:21 Paper 241b:** Environment Protection in Dangote Fertilizer Plant, Lagos Nigeria
- **8:42** Paper 241c: Evaluating Microwave-Synthesized Copper Oxide Nanoparticles from Copper Chloride with Antimicrobial Properties Using Life Cycle Assessment Techniques
- **Shishir V Kumar**, Adarsh Bafana, Si Amar Dahoumane, Liv Haselbach, Clayton Jeffryes
- **9:03** Paper 241d: Towards Sustainable Energy Mixes: Incorporating Planetary Boundaries into Energy Systems Models *Ibrahim M. Algunaibet, Carlos*
- Ibrahim M. Algunaibet, Carlos
 Pozo Fernández, Ángel Galán Martín,
 Mark A.J. Huijbregts, Niall Mac Dowell,
 Gonzalo Guillén-Gosálbez

(242) Advances in Nuclear Separation Processes and Applications

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Discovery 43 Reid Peterson, Chair Jack D. Law, Co-Chair

Sponsored by: Nuclear Engineering Division

- **8:00** Paper 242a: Cesium Removal from Tank Waste Simulants Using Crystalline Silicotitanate at 12% and 100% Bed Heights
- Amy Rovira, Sandra Fiskum, Jarrod Allred, Heather Colburn, Margaret Smoot, Andrew Carney, Reid Peterson
- **8:18** Paper 242b: Mesofluidic Exclusion of Large Particles for Nuclear Waste Applications
- **Leonard Pease**, Carolyn A. Burns, Timothy Veldman, Jason Serkowski, Nathan Phillips, Richard C. Daniel, Michael J. Minette, Xiao Ying Yu, Matthew Fountain
- 8:36 Paper 242c: Particle Back Transport Mechanisms in Crossflow Filtration with Nuclear Waste Simulants — Philip P. Schonewill, Richard C. Daniel, Carolyn A. Burns, Rick W. Shimskey, Reid A. Peterson
- **8:54** Paper 242d: A Convective-Diffusive Formulation for Crossflow Filtration of Nuclear Defense Wastes Richard Daniel, Philip P. Schonewill, Reid A. Peterson
- **9:12 Paper 242e:** Design and Testing of an Iodine and Tritium Capture System for Used Nuclear Fuel Tritium Pretreatment Processes
- **Robert Jubin**, Barry Spencer, Stephanie Bruffey
- **9:30** Paper **242f**: Aging Kinetics of Ag-Exchanged Mordenite and Ag-Functionalized Silica Aerogel in the Presence of Off-Gas Streams
- **Seungrag Choi**, Yue Nan, Alexander Wiechert, Austin Ladshaw, Sotira Yiacoumi, Costas Tsouris, Lawrence L. Taylarides
- **9:48 Paper 242g:** Towards Inverse Design of Nanoporous Materials for Isotope Separation
- Musen Zhou, Jianzhong Wu

10:06 Paper 242h: Blind Source Separation in Raman and ATR-FTIR Spectroscopy: A Processing Case Study — Giovanni Maria Maggioni, Stefani Kocevska, Ronald W. Rousseau, Martha A. Grover

(243) Advances in Process Control Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 25 Helen Durand, Chair

Xiaonan Wang, Co-Chair

Sponsored by: Systems and Process Control

- **8:00** Paper 243a: Optimal Subsystem Decomposition of Process Networks for Distributed State Estimation Based on Weighted Graph
- **Langwen Zhang**, Xunyuan Yin, Jinfeng Liu
- **8:19** Paper **243b**: Data-Driven Nonlinear Stabilization Using Operator-Theoretic Lyapunov-Based Model Predictive Control
- **Abhinav Narasingam**, Joseph Sang-II Kwon
- **8:38** Paper 243c: Passivity of Multi-Phase Reaction Systems at Chemical Equilibrium
- Zicheng Cai, B. Erik Ydstie
- **8:57 Paper 243d:** Learning and Adapting Model Predictive Controllers with Reinforcement Learning for Time-Varying Systems
- Elijah Hedrick, Katherine Reynolds, Parikshit Sarda, Debangsu Bhattacharyya, Stephen E. Zitney, Benjamin P. Omell
- **9:16** Paper 243e: Model-Based Output Feedback Control of Networked Process Systems with Event-Triggered Parameter Re-Identification
- **Amr Zedan**, Nael H. El-Farra
- **9:35 Paper 243f:** Decompositions to Handle Disparate Time-Scales in Economic Model Predictive Control
- Matthew J. Ellis
- 9:54 Paper 243g: A Deep Learning-Based Approach for Explicit Offset-Free Tracking Nonlinear Model Predictive Control
- Joel Paulson**, Ali Mesbah**
- **10:13 Paper 243h:** Lyapunov Stability and Process Flexibility Analysis: Analogies and New Approaches
- Wentao Tang, Prodromos Daoutidis

(244) Advancing into Academic Leadership

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom K Whitney L. Stoppel, Chair Sipho C. Ndlela, Co-Chair Susan C. Roberts, Co-Chair

Sponsored by: Women in Chemical Engineering Committee (WIC)

(245) Applications in Sensors: Biomedical

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Celebration 10
Kevin J. Cash, Chair
Yi Zhang, Co-Chair
Dongmei (Katie) Li, Co-Chair

Sponsored by: Sensors

- **8:00** Paper **245a**: Invited: Sensor Applications in Bioengineering: Detection of Small Molecules within Complex and Three-Dimensional Biological Milieu
- Jennie Leach
- **8:25 Paper 245b:** Tissue-like Neurochemical Sensors Operating in Brain and Gut
- **Jinxing Li**, Zhenan Bao
- **8:42** Paper 245c: Cell-Based Electrochemical Sensors for Environmental Pollutant Detection *Ariel Furst*
- **8:59** Paper 245d: Biomimetic Composites As Microfabricated, Flexible, Degradable Electrochemical Sensors *Meng Xu*, *Sayantan Pradhan*, *Ramendra Pal*, *Vamsi K*. *Yadavalli*
- **9:16 Paper 245e:** Nanopore Based Highly Sensitive and Accurate Detection of HIV
- Chang Liu, Xiaojun Wei
- **9:33 Paper 245h:** Wireless, Soft, Skin-integrated Microfluidic Systems for Electrochemical/Colorimetric Biosensing and Capture of Sweat
- Amay J. Bandodkar, John A. Rogers
- **9:50 Paper 245f:** The Electrochemical Impedance Response of a Continuous Glucose Monitor
- **Ming Gao**, Rui Kong, Mark E. Orazem
- **10:07 Paper 245g:** Measurement of Dynamic Mechanical Properties of Hydrogels Using Piezoelectric-Excited Millimeter Cantilever Sensors
- **Alexander P. Haring**, Miharu Koh, Blake Johnson

(246) Applications of Data Science in Catalysis and Reaction Engineering I Tuesday, Nov 12, 8:00 AM

Hyatt Regency Orlando, Peacock Spring

Zachary Ulissi, Chair Srinivas Rangarajan, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

- **8:00** Paper 246a: Impact of Uncertainty Quantification and Density Functional Theory Error Propagation on Surface Catalyzed Kinetic Models
- **Gerhard R. Wittreich**, Dionisios G. Vlachos, Markos A. Katsoulakis
- **8:18** Paper 246b: Automated Machine Learning and Microfluidics-Based Study and Optimization of Zeigler-Natta Catalysts
- **Benjamin Rizkin**, Ryan L. Hartman

- **8:36** Paper 246c: Simultaneous
 Canonical Polyadic Decomposition As
 a Data Fusion Algorithm to Develop
 Pseudo-Chemistry from Spectral Data
 Anjana Puliyanda, Arno De Klerk,
 Zukui Li, Vinay Prasad
- **8:54** Paper 246d: Bridging the Synthesis-Surface Information Gap: Incorporating Spectroscopy Data into an Experimental Machine Learning Framework
- **Travis Williams**, Katie McCullough, Jochen Lauterbach
- **9:12** Paper 246e: Machine Learning and Transition Metal Chemistry: Data-Driven Comparisons of First and Second Row Complexes
- Jon Paul Janet, Daniel Harper, Naveen Arunachalam, Aditya Nandy, Chenru Duan. Heather J. Kulik
- **9:30** Paper 246f: Active Machine Learning Model for the Discovery of Novel Material Systems and Its Application to Electrocatalysis
- Raul Flores, Chris Paolucci, Michal Bajdich, Ankit Jain, Muratahan Aykol, Jens K. Norskov, Thomas Bligaard
- **9:48** Paper **246**g: A Machine Learning Framework for the Analysis and Prediction of Catalytic Activity from Experimental Data
- **Alexander Smith**, James Dumesic, George W. Huber, Victor M. Zavala
- 10:06 Paper 246h: Graph Convolutional Machine Learning Methods for the Predictions of Adsorption and Thermochemistry and Surface Stability
- Seoin Back, Aini Palizhati, Wen Zhong, Nianhan Tian, Kevin Tran, **Zachary Ulissi**

(247) Applications of Molecular Modeling to Study Interfacial Phenomena II

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Rock Spring I/II Vance Jaeger, Chair Harold W. Hatch, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

- **8:00** Paper 247a: Influence of Interfaces on the Structural Evolution in Ionic Liquid-Ionic Liquid Mixtures

 Jindal K. Shah
- **8:30** Paper 247b: Interfacial Structure of Ionic Liquids Studied with Coarse-Grained Molecular Dynamics

 Tyler D. Stoffel, Justin B. Haskins,
- John W. Lawson, Sergiy Markutsya
 8:45 Paper 247c: Spatially Varying
 Chemical and Physical Properties
 Modulate Interfacial Hydrophobicity of
- Self-Assembled Monolayers

 Bradley C. Dallin, Hongseung Yeon,
 Nicholas L. Abbott, Reid C. Van Lehn

- **9:00** Paper **247d:** The Protein Surface Hydrophilic Lipophilic Balance As a New Approach for Characterizing Large Biosurfactants
- Juliana Erika Cristina Cardona Jaramillo, **Luke E. K. Achenie**, Oscar Alberto Alvarez, Andrés Fernando González Barrios
- **9:15 Paper 247e:** Conformational and Dynamical Behaviors of Polyelectrolytes Under Spatial and Dielectric Confinement
- **Trung Nguyen**, Monica Olvera de la Cruz
- **9:30 Paper 247f:** Gibbs Ensemble Monte Carlo Simulations for Additive Loading in Surfactant Bilayers
- **Mona Minkara**, Connor Venteicher, J. Ilja Siepmann
- **9:45** Paper 247g: Understanding the Role of Cellulose Nanocrystals As Novel Shale Hydration Inhibitors for Water-Based Drilling Fluids
- **Andres Vodopivec**, Francisco R. Hung

10:00 Paper 247h: Molecular-Level Characterisation of Crystal/Solution Interfaces: The Case of Ibuprofen
— Veselina Marinova, Matteo
Salvalaglio

10:15 Paper 50i: Molecular Simulation-Guided Design of Hydrophilic-Hydrophobic Interfaces for Hybrid MOF Microtanks for Methane Storage

— Ryther Anderson, Bomsaerah Seong, Moises A. Carreon, **Diego Gomez Gualdron**

(248) Area Plenary: Area 8A Emerging Areas in Polymer Science and Engineering I (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 5 Muzhou Wang, Chair Allie Obermeyer, Co-Chair

Sponsored by: Polymers

8:00 Paper 248a: Molecular Engineering Approaches to Adaptive Polymers

- Stuart J. Rowan

8:35 Paper **248b:** Processable Multiple Network Composite Design Using Insights from Sequential IPNs

- Meredith Wiseman

9:10 Paper 248c: Engineering Lubricating Polymers Under Extreme Conditions Using Polymer Architecture

- Matthew E. Helgeson

9:45 Paper 248d: Direct Measurement of the Local Glass Transition in Diblock Copolymers and Nanocomposites

- Rodney D. Priestley

(249) Area Plenary: Bionanotechnology (Invited Talks)

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Discovery 45
Lorraine Leon, Chair
Elizabeth Nance, Co-Chair
Catherine A. Fromen, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 249a: Collecting Interstitial Fluid from the Skin As a Novel Source of Biomarkers

- Mark R. Prausnitz

8:50 Paper **249b:** From Drug Self-Assembly to Supramolecular Medicine — *Honggang Cui*

9:40 Paper 249c: Nanotechnology-Based Probes of Structure-Function in Living Tissue

— Elizabeth Nance, Chad D. Curtis, Michael McKenna, Rick Liao, Jeremy Filteau

(250) Area Plenary: Interfacial Phenomena (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom J Raymond Tu, Chair Marina Tsianou, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 250a: Interfacial Processing and Engineering of Multicomponent Adsorption at Fluid-Fluid Interfaces

- Lynn M. Walker

8:50 Paper 250b: Polyelectrolyte Complex Micelles: Properties and Applications

— Matthew V. Tirrell

9:40 Paper 250c: "Cinematography" at the Nanoscale, from Colloidal Crystallization to Protein Transformation

- Qian Chen

(251) Biofuels Production: Design, Simulation, and Economic Analysis

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Regency Ballroom U

Ana I. Torres, Chair Ramalingam Subramaniam, Co-Chair Peyman Fasahati, Co-Chair

Sponsored by: Sustainable Biorefineries

- **8:00** Paper **251a**: Carbon Negative Biofuel and Power Systems Via Hybrid Pyrolysis and Anaerobic Digestion Biorefineries
- **Alvina Aui**, Arna Ganguly, Irene Mas-Martin, Mark Mba Wright
- **8:25 Paper 251b:** Synthesis and Analysis of Biorefinery Systems with Novel Lignin and Stillage Valorization Technologies
- **Kefeng Huang**, Peyman Fasahati, Rex T. L. Ng, Christos T. Maravelias
- **8:50 Paper 251c:** Biomass-Derived Liquid Fuels Via Fischer-Tropsch Process As a Potential Replacement for Marine Fuels
- Eric CD Tan, Ling Tao, Mary Biddy
- **9:15 Paper 251d:** Exploring Sustainable n-Butanol Production By *Rhodopseudomonas Palustris* TIE-1

— **Wei Bai**, Tahina Ranaivoarisoa, Karthikeyan Rengasamy, Rajesh Singh, Arpita Bose **9:40** Paper 251e: Process Design and Economic Analysis of Ethanol and Diesel Production from Genetically Modified Lipid-Accumulating Sorghum

— Peyman Fasahati, J. Jay Liu, Christopher M. Saffron

(252) Biomass Characterization, Pretreatment, and Fractionation

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Discovery 47 Zhihua Jiang, Chair Zhaohui Tong, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

8:00 Paper 252a: Discrete Element Modeling of Granular Flow of Flexible Woody Biomass Particles

— **Yidong Xia**, Zhengshou Lai, Tyler L. Westover, Jordan Klinger, Hai Huang, Qiushi Chen

8:25 Paper 252b: Solvent and Processing Conditions for Pretreatment and Dissolution of Cellulose

— **Mohammad Ghasemi**, Marina Tsianou, Paschalis Alexandridis

8:50 Paper **252c:** Effectiveness of Cotreatment during Fermentation on Various Feedstocks, Impact on Different Microbes, and Milling Energy Requirements

— **Sanchari Ghosh**, Mikayla L. Balch, Galen D. Moynihan, Evert K. Holwerda, Brenden P. Epps, Lee R. Lynd

9:15 Paper 252d: Influence of Industrial Fractionation Methods on Lignin Structure

— Andrew W. Tricker, Thomas T. Kwok, Michael Stellato, Nicholas S. Kruyer, Matthew J. Realff, Andreas S. Bommarius, Carsten Sievers

9:40 Paper 252e: Molecular Reconstruction of Esterified Pyrolysis Bio-Oil Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

— Claudia X. Ramirez, Juan E. Torres, Diana Catalina Palacio Lozano, Mark P. Barrow, Rafael Cabanzo, Enrique Mejia-Ospino

10:05 Paper 252f: Catalytic Hydrothermal Treatment (CHT) of Lignocellulosic Biomass

— Anuj Thakkar, Katelyn Shell, Martino Bertosin, Dylan Rodene, **Vinod S. Amar**, Bharat Maddipudi, Tylor Westover, Sandeep Kumar, Alberto Bertucco, Ram B. Gupta, Rajesh Shende

(253) Breakthroughs in C1 to Chemicals and Processing Engineering

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Regency
Ballroom Q
Zhongmin Liu, Chair
Emily Cole, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

8:00 Paper **253a**: Innovative Fluidized Bed Technologies in Coal to Chemical Processes

— **Mao Ye**, Tao Zhang, Jinling Zhang, Zhongmin Liu

8:25 Paper 253b: Methyl Formate Hydrogenation to Higher Hydrocarbons over Mn- and Ti-Oxide Promoted Cobalt Catalysts

— **Andrew Raub**, Motahare Athariboroujeny, Norbert Kruse

8:50 Paper 253c: Gallate-Based Metal-Organic Framework As a Heterogeneous Catalyst for the Coupling of CO₂ and Epoxides — *Min Yi*, *Zhiguo Zhang*, *Zongbi Bao*,

Qiwei Yang, Yiwen Yang, Ren Qilong

9:15 Break

9:40 Paper 253d: Biological Upgrading of Methane for the Production of Chemicals and the Techno-Economic Analysis

— Qiang Fei, Bobo Liang, Rongzhan Fu

10:05 Paper 253e: In-Situ Hydrogen Sulfide Removal and Biogas Upgrading Via a One-Reactor System Integrating Solid-State Anaerobic Digestion of Food Waste and Bioelectrochemical

- Lingkan Ding, Yan Chen, Bo Hu

(254) Challenges in Entrepreneurship: Ensuring Success for your Start-up

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom N Henry Uyeme, Chair

Sponsored by: Entrepreneurship in Chemical Engineering - Sponsored by CIEE

12:30 Paper 254a: Remarks by Praful Krishna, CEO, Coseer — *Praful Krishna*

12:40 Paper 254b: Remarks by Jason Zeng, Entrepreneur, PhD Student, Montana State University
— Jason Zeng

12:50 Paper **254c**: Remarks by Jessica Ocampos, CEO, Camnexus — *Jessica Ocampos*

1:00 Paper 254d: Remarks by Frana James, CEO, Allied Microbiota — *Frana James*

1:10 Paper 254e: Remarks by George Diloyan, CEO, Nanotech Industrial Solutions

— George Diloyan

1:20 Panel Discussion

(255) Colloidal Hydrodynamics

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Orlando
Ballroom L

James Swan, Co-Chair Travis W. Walker, Co-Chair

Sponsored by: Fluid Mechanics

- 8:00 Paper 255a: The Hydrodynamic Force on a Slender Particle Executing Oscillatory Translation in Unsteady Stokes Flow
- Jason K. Kabarowski**, Aditya S. Khair**
- **8:15** Paper 255b: On the Viscosity of Adhesive Hard Sphere Dispersions: Critical Scaling and the Role of Contact Mechanics
- James Swan
- 8:30 Paper 255c: The Colloidal Hydrodynamics of Intracellular Transport — Roseanna N. Zia, Akshay Maheshwari, Drew Endy, Emma Gonzalez, Alp Sunol
- **8:45** Paper 255d: Connecting Microscopic Dynamics and Macroscopic Properties of Soft Particle Glasses *Fardin Khabaz*, *Stefania Traettino*,
- Michel Cloitre, Roger T. Bonnecaze
- **9:00 Paper 255e:** Active Particles Powered By Quincke Rotation Instability in a Bulk Fluid
- **Debasish Das**, Eric Lauga
- **9:15** Paper 255f: Hydrodynamic Interactions Effect on the Aggregation of Colloidal Dispersions in the Presence of Sedimentation
- Marco Lattuada
- **9:30 Paper 255g:** Electrostatics and Friction in Dense Suspensions of Rough Colloids
- Lilian Hsiao
- **9:45** Paper **255h**: Translational and Rotational Diffusion of Polymer Grafted Nanoparticles in Synovial Fluid and Hyaluronan Solutions
- Mythreyi Unni, Lorena Maldonado-Camargo, Shehaab Savliwala, Brittany Partain, Kyle Allen, Carlos Rinaldi, Suresh Narayanan, Alec Sandy, Qingteng Zhang, Eric M Dufresne, Pawel Grybos, Anna Koziol, Piotr Maj, Robert Szczygiel
- **10:00 Paper 255i:** Deformation Dynamics of Paramagnetic Colloidal Clusters in Time-Varying Fields
- **Kedar Joshi**, Elaa Hilou, Sibani Lisa Biswal
- **10:15 Paper 255j:** Dynamic Simulations and Rheological Studies of Suspensions of Magnetic Particles
- Mingyang Tan, Joshua A. Adeniran, Christopher Beal, **Travis W. Walker**

(256) Computational Studies of Self-Assembly

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Silver Spring

Julia Dshemuchadse, Chair Sumit Sharma, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 256a: Nonequilibrium Associative Retrieval of Multiple Stored Self-Assembly Targets

— Gili Bisker

- **8:15 Paper 256b:** Hard Superellipses: Phase Behavior & Structures
- Isaac Torres-Diaz, Michael A. Bevan
- **8:30 Paper 256c:** Impact of Size Disparity on Assemblies from Multi-Flavored Particles
- **Runfang Mao**, Evan Pretti, Jeetain Mittal
- **8:45** Paper **256d:** Thermodynamic Phase Behaviors and Kinetic Pathways for Entropic Self-Assembly of Bipyramids
- **Yein Lim**, Sangmin Lee, Sharon C. Glotzer
- **9:00** Paper 256e: Structural Development during Emulsion Assembly of Binary Particle Mixtures: Simulation and Experiment
- **Thomas Gartner III**, Christian Heil, Arthi Jayaraman
- **9:15** Paper 256f: Investigating the Self-Assembly and Structure of Nanoparticles Containing Curved Carbons
- **Kimberly Bowal**, Jacob W Martin, Laura Pascazio, Markus Kraft
- **9:30 Paper 256g:** Self-Assembly of Adsorbed Surfactant Molecules at Metal-Water Interfaces
- Xueying Ko, Sumit Sharma
- **9:45** Paper 256h: Molecular Modelling of Hydrophobic Ion Pairing Self Assembly for Nanoprecipitation: From Explicit Solvent United-Atom to Implicit Solvent Coarse Grain Simulations
- **Daniel J. Kozuch**, Kurt D. Ristroph, Robert K. Prud'homme, Pablo G. Debenedetti
- 10:00 Paper 256i: Nano-Structured Films of Semifluorinated Alkanes "Primitive Surfactants": Formation and Size of Hemi-Micelles By Molecular Dynamics
- Gonçalo M. C. Silva, Pedro Morgado, Michel Goldmann**, Eduardo Filipe**
- **10:15** Paper **256**j: Self-Assembly of Quorum Sensing Signal Molecules *Samarthaben J. Patel, Curran Gahan, Helen E. Blackwell, David M.*

Lynn, Reid C. Van Lehn

(257) Concentrated Solar for Power Generation and Chemical Processing

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Regency Ballroom T

Nick AuYeung, Chair Christopher L. Muhich, Co-Chair Ashley M. Pennington, Co-Chair Wojciech Lipinski, Co-Chair Alexandre Yokochi, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 257a: Experimental Investigation of YMnO₃ Perovskites with Sr a-Site and Al B-Site Doping for Solar Thermochemical Fuel Production — Richard Carrillo, Jonathan R. Scheffe

- **8:25** Paper 257b: Understanding the Oxidation Kinetics Mechanism of Ceria Based Materials in Solar Thermochemical Gas Splitting
 Steven Wilson, Bennett Mandal, Christopher L. Muhich
- **8:50** Paper 257c: Functional Ceramics for Solar Thermochemical Storage, Hydrogen and Liquid Fuel Production *Dorottya Guban, Josua Vieten,*
- Stefan Brendelberger, Martin Roeb, Christian Sattler
- **9:15** Paper 257d: A Comparison of Solid-Gas Thermochemical Energy Storage Reactions and Process Configurations for CSP Applications *Xinyue Peng, Thatcher W. Root,*

Christos T. Maravelias

- **9:40** Paper **257e**: Flexible Heat Integration to Enhance Solar Energy Utilization in a Hybrid CSP Plant *Kevin Ellingwood*, *Kody M. Powell*
- 10:05 Paper 257f: Heliostat and Solar
- Simulator for Solar Thermal Applications
 Yu Miao, Chenguang Li, Suzanne
 Acton, Chibuikem Agwamba, Avery
 Heidemann, Connor Nahrgang, Luke
 Parker, Annette von Jouanne, Alexandre
 Yokochi

(258) Conceptual Process Design in Refining, Petrochemicals and Gas Processing

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Challenger 38/39

Shu Wang, Chair Yu-Jeng Lin, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

- **8:00** Paper 258a: KBR's Propane Dehydrogenation Technology (K-PRO) Meets Market-Driven on-Purpose Propylene Demand
- Jeff Caton
- **8:21 Paper 258b:** Process Conceptualization in a Carbon-Constrained World: Leveraging Optimization and Systems Engineering to Balance Multiple Objectives
- Tony Joseph Mathew, Amrit Jalan, Chris Goheen, Gary Kocis, Sundar Narayanan, Linlin Yang, Mohit Tawarmalani, Rakesh Agrawal
- **8:42 Paper 258c:** Dynamic Simulation Studies for Optimal Design and Operation of an LNG Liquefaction Process
- Mozammel Mazumder, Qiang Xu
- **9:03 Paper 258d:** Crude Oil-to-Chemical Conceptual Design *Andrew W. Sloley*
- **9:24 Paper 258e:** Design of a Single Wall Divided Wall Column for the Separation of an Industrial Quaternary Mixture
- Tanmay Kakade

- 9:45 Paper 258f: Process Intensification in the Methanol-to-Propylene Process Enabled By Rigorous Kinetics Lin Lin, Felix Warnecke, Stéphane Haag, Thomas Renner, Christopher Drosdzol, Hannsjörg Freund
- **10:06** Paper **258g:** Oxidative Dehydrogenation for the Conversion of Ethane to Ethylene
- **Gennaro J. Maffia**, Xufang Liu, Amanda Peterman, Anne Gaffney

(259) Data Science & Analytics for Operations Support and Predictions in Pharmaceutical Processes & Products

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 6 Shekhar Viswanath, Chair XiaoXiang Zhu, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **8:00** Paper **259a**: Data Rich Experimentation and Machine-Assisted Process Development for Rapid Reaction Optimization
- **Jonathan P. McMullen**, Jon Jurica, Shane Stone
- **8:21** Paper 259b: Optimal Time Sampling Strategy in Pharmaceutical Reactions for the Estimation of Accurate DRSM Models
- **Yachao Dong**, Christos Georgakis, Jason Mustakis, Joel M. Hawkins, Jonathan McMullen, Kevin Stone
- **8:42 Paper 259c:** Expedite Particle Engineering Process Development Using Data Science
- **Tiago Porfirio**, Ines Matos, João Vicente, Viriato Semião
- **9:03 Paper 259d:** Data-Driven CLD-to-Psd Model for in-Line Crystal Size Monitoring
- **Roberto Irizarry**, Akshaya Nataraj, Jochen Schoell, Eric Sirota, Aaron Cote
- 9:24 Paper 259e: Kernel Mean Embedding of Distributions: A New Data-Driven Model Approach for Modelling a Continuous Pharmaceutical Twin-Screw Granulation Process — Daan Van Hauwermeiren, Michiel

Stock, Thomas De Beer, Ingmar Nopens

- 9:45 Paper 259f: Breaking Force and Disintegration Prediction of Tablet Formulations Using Machine Learning — Ilgaz Akseli, Chris MacTaggart, Catherine Guarino, Jianmin Li
- **10:06 Paper 259g:** Development of Data-Driven and Hybrid Models for Continuous Pharmaceutical Manufacturing Lines Under Industry 4.0 Framework
- Yingjie Chen, Marianthi lerapetritou

(260) Development of Pharmaceutical Process Control Strategies for Drug Product Manufacture

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Celebration 8
Huiquan Wu, Chair
Brian C. Anderson, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **8:00 Paper 260a:** Determination and Understanding of Dynamic Lead Lag between in-Line NIR Tablet Press Feed Frame and Off-Line NIR Tablet Measurements
- Michiel Peeters, Elisabeth Peeters, Fien De Leersnyder, Daan Van Hauwermeiren, Giuseppe Cogoni, Yang Liu, Thomas De Beer
- 8:21 Paper 260b: Digitalization in Active Process Control of Pharmaceutical Continuous Manufacturing of Oral Solid Dosage *Qinglin Su*, Alessandra E. Anderson-Lewis, Sudarshan Ganesh, Yasasvi Bommiready, Marcial Gonzalez, Gintaras Reklaitis, Zoltan K. Naay
- **8:42 Paper 260c:** Real-Time Monitoring and Model-Based Prediction of Product Properties in a Dropwise Additive Manufacturing Process for Pharmaceuticals
- **Andrew J. Radcliffe**, Zoltan K. Nagy, Gintaras V. Reklaitis
- **9:03** Paper 260d: Process Control Strategy Development for a Challenging Drug Powder Blending Process Via Real-Time Process Analytical Technology (PAT) Monitoring and Prediction
- **Huiquan Wu**, Suyang Wu, Alpa Patel, Koushik Sowrirajan
- **9:24 Paper 260e:** Advanced Control Strategies for a Continuous Tableting Line Via Hot Melt Extrusion
- **Stephan Sacher**, Selma Celikovic, Jakob Rehrl, Johannes Poms, Martin Kirchengast, Julia Kruisz, Martin Sipek, Sharareh Salar-Behzadi, Hannes Berger, Gerald Stark, Martin Horn, Johannes G. Khinast
- **9:45** Paper **260f**: Exploring the Robustness of Terahertz-Based at-Line Porosity Measurements for Realising a Non-Destructive Dissolution Assay of Tablets during Manufacturing
- **Prince Bawuah**, Daniel Markl, Daniel Farrell, Mike Evans, Alessia Portieri, Andrew Anderson, Daniel Goodwin, Ralph Lucas, Axel Zeitler
- **10:06 Paper 260g:** Commercial Control Strategy Development for a High Shear Wet Granulation Process
- **Carl Knable**, Kathleen Apfelbaum, Todd McDermott

(261) DORIC: Supporting Our Students with Disabilities

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 31 Christopher Pope, Chair

Sponsored by: Engineering for Inclusion

(262) Dynamics and Modeling of Particles, Crystals and Agglomerate Formation

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 21 Priscilla J. Hill, Chair Eirini Goudeli, Co-Chair

Sponsored by: Particle Production and Characterization

- **8:00 Paper 262a:** Prediction of Nanoparticles Size Distribution: The Effects of Ligand Surface Coverage and Nanoparticle Size in Altering the Kinetics of Surface Growth
- **Saeed Mozaffari**, Wenhui Li, Mudit Dixit, Giannis Mpourmpakis, Ayman M. Karim
- 8:25 Break
- **8:50 Paper 262c:** Quantification and Control of Amorphous Contents By Raman. Applications and Case Studies in Pharmaceutical Processing
- Michelle Raikes, Fredrik Nordstrom
- **9:15** Paper 262d: Breakage Kinetics of Urea Crystals in Agitated Slurries

 Priscilla J. Hill
- 9:40 Paper 262e: Photoelastic Properties of 3D Printed Particles — Negin Amini, Karen P. Hapgood, David Morton, Jun Zhang

(263) Computing for ChEs: Teaching Programming and Simulation Software

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 29/30 Eva Sorensen, Chair Manuela A.A. Ayee, Co-Chair

Sponsored by: Undergraduate Education

- **8:00 Paper 263a:** Teaching Aspen Plus Via Student-Developed Video Modules
- Daniel D. Burkey, Jennifer Pascal
- **8:18 Paper 263b:** Integration of Aspen Plus® Videos into the Chemical Engineering Curriculum at the University of Kansas
- Michael Shao, Mark B. Shiflett
- **8:36 Paper 263c:** Teaching Chemical Engineering Fundamentals with Comsol Multiphysics®
- William M. Clark
- **8:54** Paper **263d:** Smart Computing in Undergraduate Courses Improved Understanding of Fundamentals
- Satish J. Parulekar
- **9:12** Paper **263e:** Integrated Molecular Modeling Education in the Chemical Engineering Curriculum
 - Peter J. Ludovice, David MacNair

- **9:30 Paper 263f:** Combining Various Software Tools for Enhancing Programming and Numerical Problem Solving Capabilities
- Mordechai Shacham, Michael B. Cutlip
- **9:48** Paper 263g: A Scaffolded Approach to Process Modeling Education with Literate Programming Tools
- **Stuart W. Prescott**, Francisco J. Trujillo
- **10:06 Paper 263h:** Introducing Chemical Engineers to Coding, Data and Visualization through Matlab
- Jason E. Bara, Vincent Scalfani

(264) Functional Nanoparticles Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 20 Xing Yangchuan, Chair Da Deng, Co-Chair

Sponsored by: Nanoparticles

- **8:00 Paper 264a:** Investigating the Properties of Nanoparticles Containing Fullerene-like Molecules
- **Kimberly Bowal**, Jacob W Martin, Laura Pascazio, Markus Kraft
- **8:15** Paper **264b:** Ultrasonic Spray Delivery of Precursors for Laser Pyrolysis Synthesis of Nanoparticles
- **Mohammad Malekzadeh**, Parham Rohani, Mark T. Swihart
- **8:30** Paper **264c:** Tailoring the Bioactivity of Flame-Made Nanoparticles for Surgical Applications
- Martin T. Matter, Fabian Starsich, Andrea Schlegel, Sotiris E. Pratsinis, Inge K. Herrmann
- **8:45** Paper 264d: Corrosion Protection of Epoxy Coating with Calcium Phosphate Encapsulated By Mesoporous Silica Nanoparticles
- **Zoi Lamprakou**, Huichao Bi, Claus Erik Weinell, Kim Dam-Johansen
- **9:00 Paper 264e:** Self-Assembled Nanoparticle Antireflection Coatings on Geometrically Complex Optical Surfaces
- **Peng Jiang**, Calen Leverant
- 9:15 Intermission
- **9:20 Paper 264f:** Electronic Structure of Cu₂-Xse Nanoparticles for Plasmonic Catalysis: A Density Functional Theory Study
- Daniel Harper, **Jonathan Ruffley**, Jonathan Klan, J. Karl Johnson
- **9:35 Paper 264g:** Application of Carbon Nanotube & Cellulose Nanocrystal Composite in Conducting Films
- **Zachariah Pittman**, Christopher L. Kitchens
- **9:50** Paper **264h**: Influence of Defect Microstructure on the Structural Color of Colloidal Films
- Tianyu Liu, **Bryan Vansaders**, Sharon C. Glotzer, Michael J. Solomon

- **10:05** Paper **264i**: MoS₂-Pt Deposited on Nitrogen-Doped Carbon Nanotubes As Efficient Electrocatalyst for Hydrogen Evolution Reaction
- Alejandra de la Rosa Goméz, Juan D. Frías Hernandez, Nicté J. Perez-Viramontes, M. Luisa García-Batancourt, Sergio M. Duron-Torres, ismailia L. Escalante-Gacia
- **10:20 Paper 264j:** Combustion Synthesized Nickel-Cobalt Catalyst Deactivation By Coking during Ethanol Decomposition Reaction
- **Anchu Ashok, Anand Kumar**, Faris Tarlochan

(265) Fundamentals of Catalysis III: Hydrogenation and Dehydrogenation

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom D Prashant Deshlahra, Chair Thomas P. Senftle, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper 265a: Sensitivity of Surface Structures Towards Hydrodeoxygenation of Propanoic Acid over Palladium Catalysts
- Andreas Heyden, **Subrata Kumar Kundu**
- **8:18** Paper 265b: Crowding and Curvature: Nanoparticle Models Revisited for Chemisorption and Hydrogenolysis Reactions
- **Abdulrahman Almithn**, Ibrahim Alfayez, David Hibbitts
- **8:36 Paper 265c:** Kinetic Fingerprints of Subsurface Hydrogen Active in Hydrogenation
- Andrew J. Gellman, Irem Sen
- **8:54** Paper **265d**: Selective Hydrogenation of Acetylene over Cu-Pd and Ag-Pd Catalysts
- **Madelyn R. Ball**, Edgard A. Lebron, Samantha F. Ausman, Cole W. Hullfish, James A. Dumesic
- **9:12** Paper 265e: Chemical Identity of Hydrogen Species on Sulfided Ruthenium: A Combined Theoretical and Experimental Work
- **Roberto Schimmenti**, Haiting Cai, Haoyu Nie, Ya-Huei (Cathy) Chin, Manos Mavrikakis
- **9:30** Paper 265f: Control of Surface Reactivity Towards Unsaturated C-C Bonds and H over Ni-Based Intermetallic Compounds in Semi-Hydrogenation of Acetylene
- Yuanjun Song, Siris Laursen
- **9:48 Paper 265g:** First Principles Analysis of Selectivity and Durability of Pt-Based Alloys for Light Alkane Dehydrogenation
- **Yinan Xu**, Ranga Rohit Seemakurthi, Zhenwei Wu, Jeffrey T. Miller, Jeffrey Greeley

10:06 Paper **265h**: Cobalt Oxide Supported on SiO₂ Modified Al₂O₃ for Propane Dehydrogenation: High Cobalt Oxide Dispersion and Enhanced Selectivity

— **Nikita Dewangan**, Madhav Sethia, Hidajat Kus, Sibudjing Kawi

(266) How We Teach: Ethics, Teamwork, Leadership, and Professional Skills

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 23 Christy Wheeler West, Chair Daniel D. Burkey, Co-Chair

Sponsored by: Undergraduate Education

8:00 Paper 266a: Teamwork and Teamwork Evaluation Skills — *Jennifer Cole*

8:20 Paper 266b: Using the Trolley Problem in Chemical Engineering Ethics Education

- Anthony Butterfield

8:40 Paper **266c:** Preparing Students for Professional Success: Cross-Disciplinary Lessons

— *Keith L. Hohn*

9:00 Paper 266d: A Novel Course Sequence on Critical Thinking.

Publishing, and Publication Ethics for Engineering Graduate Students

— *Michael A Matthews*, *Gina Kunz*, *Darin Freeburg*, *Kevin Brock*

9:20 Paper 266e: Agile Management of PhD Projects: A Risk-Mitigation Plan for Graduate Education

— **Laura Pirro**, Marina Montero Carrero, Francesco Contino, Joris W. Thybaut

9:40 Paper 266f: TA Survival Guide: Navigating Your First Week of Classes — *Molly Skinner*, Sandra L. Pettit

(267) Hydrogel Biomaterials: Dynamic and Stimuli-Responsive Hydrogels

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Celebration 16
Steven Caliari, Chair
Adrianne M. Rosales, Co-Chair
Adam Ekenseair, Co-Chair
Anita Shukla, Co-Chair

Sponsored by: Biomaterials

8:00 Paper 267a: Tuning Affinity and Network Dynamics in Supramolecular Hydrogel Biomaterials

— *Matthew Webber*

8:18 Paper 267b: Covalent Adaptable Hydrogel Networks Measured with µ2rheology to Mimic the pH Environment in the GI Tract — Nan Wu, Kelly M. Schultz

8:36 Paper 267c: Combining Shear-Thinning and Temporal Covalent Crosslinking in an Injectable Hyaluronic Acid Hydrogel

— **Victoria G. Muir**, Sarah Gullbrand, Beth Ashinsky, Robert L. Mauck, Jason A. Burdick **8:54** Paper 267d: Tunable Viscoelastic Synthetic Hydrogels Crosslinked through Reversible Thia-Conjugate Addition

— **Thomas FitzSimons**, Eric Anslyn, Adrianne M. Rosales

9:12 Paper 267e: Biomimetic Modification of Thermoresponsive Hydrogel Scaffolds for Enhanced Mucoadhesion

- Ninad Kanetkar, Adam Ekenseair

9:30 Paper 267f: Tailoring Gelation and Mechanical Properties of Fibrin-Based Extracellular Matrix Using Stimulus-Responsive Poly (Lactic-co-Glycolic Acid) Microgelator

— **Yu-Tong Hong**, Daniel T. Bregante, Johnny Ching-Wei Lee, Yongbeom Seo, Lawrence B. Schook, David Flaherty, Simon Rogers, Hyunjoon Kong

9:48 Paper **267g:** Gas-Filled Nanoscale Additives for Acoustically Responsive Hydrogel

— **Paulene Abundo**, Di Wu, Jeong Hoon Ko, Dina Malounda, Mikhail G. Shaniro

10:06 Paper 267h: Granules Enable Multiscale and Dynamic Tissue-like Behaviors in Synthetic Hydrogel

— **Yin Fang**, Yiliang Lin, Yuanwen Jiang, Endao Han, Xianghui Xiao, Jin Wang, Heinrich M. Jaeqer, Bozhi Tian

(268) IACChE's James Y. Oldshue Lecture (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom H **L. Antonio Estévez, Chair**

Sponsored by: Liaison Functions

8:00 Paper 268a: Response of Magnetic Nanoparticles to Time Varying Magnetic Fields: Ferrohydrodynamics, Nanoscale Thermal Therapy, and Magnetic Particle Imaging

— Carlos Rinaldi

(269) Industry 4.0 and Digital Transformation (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 27 Ravindra Aglave, Chair Ryan L. Hartman, Co-Chair Yash Puranik, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 269a: Introductory Remarks for the Industry 4.0 and Digital Transformation Session

— Ravindra Aglave

8:05 Paper 269b: Leading the Industry 4.0 Journey in the Manufacturing Sector with Cross-Industry Collaboration and Al-Powered Innovation

— Sam Samdani

8:35 Paper 269c: Real-Time Analytics for IIoT

— Bijan Sayyar-Rodsari

9:05 Paper **269d:** Process Optimization in the Age of Industry 4.0 — *Lorenz T. Biegler*

9:35 Paper 269e: Value-Driven Digitalization Initiatives at Dow — *Satyajith Amaran*

10:05 Paper 269f: Q&A Panel Discussion

— Sam Samdani, Bijan Sayyar-Rodsari, Lorenz T. Biegler, Satyajith Amaran

(270) In Honor of Dan Luss' 80th Birthday (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Florida Ballroom B

Michael Harold, Chair Robert W. McCabe, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 270a: Comparison of Two Auto-Thermal Multi-Fuel Mobile Reformers for H₂ Generation:the Pd-Membrane Reactor and the ICE with Heat-Recuperation

- Moshe Sheintuch

8:30 Paper **270b**: Analysis of Linear and Nonlinear Systems in Chemical Engineering Using Symbolic Computation Approaches

- Patrick L. Mills

9:00 Paper 270c: Advanced Digital Design of Pharmaceutical Manufacturing Processes

— Johannes G. Khinast

9:30 Paper 270d: Siloxane
Removal from Biogas Using a UV
Photodecomposition Technique
— Theodore Tsotsis, Alireza Divsalar,
Hasan Divsalar, Matthew N. Dods

10:00 Paper **270e**: Steady-State Multiplicity, Stability and Pattern Formation in Autothermal Reactors for Oxidative Coupling of Methane

- Balakotaiah Vemuri

(271) In Honor of Professor Ignacio Grossmann's 70th Birthday - I (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 24 Nikolaos V. Sahinidis, Chair Stratos Pistikopoulos, Co-Chair

Sponsored by: Systems and Process Design

8:00 Paper 271a: A Decade of Advances in Chemical Production Scheduling

— Christos T. Maravelias

8:21 Paper 271b: Optimization Based Polyhedral Region Approach for MULTI-CLASS DATA Classification Problem — *Metin Turkay*

8:42 Paper 271c: Process Design: Challenges Towards a Future Renewable Based Process Industry — *Mariano Martín*

9:03 Paper 271d: Quantum Computing for Process Systems Optimization and Data Analytics

- Fengqi You

9:24 Paper 271e: Branch-and-Price for a Class of Mixed-Integer Nonlinear Programs

— Qi Zhang

9:45 Paper 271f: Process System Engineering Modeling: A Software Engineering Perspective

— Melina Vidoni, Laura Cunico, Aldo Vecchietti

10:06 Paper 271g: Multi-Level Mixed-Integer Optimization, Adjustable Robust Optimization & Multi-Parametric Programming

- Efstratios N. Pistikopoulos

(272) In Honor of Prof. Yannis G. Kevrekidis' 60th Birthday (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 26 Stanislav Y. Shvartsman, Chair T. J. Mountziaris, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

8:00 Paper 272a: Hybrid Neural-Network Kalman-Bucy Filter Approach for Adaptive Tracking of Complex Signals

— Ramiro Rico-Martinez, Mario Calderon-Ramírez, Hector A Olmos Guerrero

8:19 Paper 272b: Nonlinear Dynamics of Non-Newtonian Fluids

— *Michael D. Graham*

8:38 Paper 272c: Re-Exploring Noninvertible Systems — *Raymond A. Adomaitis*

8:57 Paper 272d: Temporal and Spatial Information Processing in Natural and Engineered Biomolecular Systems

— J. Krishnan

9:16 Paper 272e: Robust Optimisation and Control of Large-Scale Nonlinear Systems: A Suite of Model-Reduction

— Constantinos Theodoropoulos

Based Methodologies

9:35 Paper 272f: Equation-Free Computation of Invariant Manifolds of Microscopic Simulators

— Constantinos Siettos, Lucia Russo

9:54 Paper 272g: Generalized S.V.D. Observers for Linear Time Invariant Systems

— **Gbolahan Dada**, Antonios Armaou

10:13 Paper 272h: Examples of Self-Similar Blowup: To Infinity and (Sometimes) Back

— Panayotis G. Kevrekidis

(273) In Honor of the 2018 Recipient of the Warren K. Lewis Award (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 22 Abraham M. Lenhoff, Co-Chair Eric M. Furst, Co-Chair

Sponsored by: Education

8:00 Introductory Remarks

8:05 Paper 273a: Tunde Ogunnaike: Teacher, Author, Researcher, Administrator

— Thomas F. Edgar

8:25 Paper 273b: Polymer Reaction Engineering in the Origins of Life:How to Get from Synthetic Rubber to Chemical Evolution

- F. Joseph Schork

8:45 Paper 273c: Estimating the State of a Dynamical System: From Kalman Filtering to Moving Horizon State Estimation

- James B. Rawlings

9:05 Paper 273d: Biological Inspiration for Network Synchronization

- Francis J Doyle III

9:25 Paper 273e: Deep Knowledge Versus Deep Learning

— **Derrick K. Rollins Sr.**, Parnian Ghasemi

9:45 Paper 273f: Enhancement of Chemical Engineering Education through Design Thinking: Integration of Theory and Cyber-Assisted Methods

- Kirti M. Yenkie

10:05 Paper **273**g: The Manifest Fingerprints of Excellence in Education and Mentoring

- Marc R. Birtwistle

(274) Innovations in Production of Unconventional Reservoirs

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Challenger 40 Sandeep Verma, Chair Andrey Filippov, Co-Chair

Sponsored by: Upstream Engineering and Flow Assurance Forum

8:00 Paper 274a: Converting Low-Pressure Natural Gas to Foamed Stimulation Fluid: Defining the Operating Envelope

— **Sandeep Verma**, Alhad Phatak, Piyush Pankaj

8:25 Paper **274b:** Impact of Zirconia Nanoparticles and Polymer on Drilling Fluid Rheology, Fluid Loss and Filter Cake Properties

— Mamdouh A. Al-Harthi, **Muhammad Shahzad Kamal**, Hafiz Ahmad

8:50 Paper 274c: Brine-Soluble Zwitterionic Polymers with Tuneable Adsorption on Carbonates

— Mohammed Kawelah, Yuan He, **S. Sherry Zhu**, Ayrat Gizzatov, Timothy Swager

9:15 Paper 274e: Green Solvent for Enhanced Recovery in Unconventional Resources

— **Sandeep Verma**, Andrew E. Pomerantz, George Waters, Kyle Bake, Griffin Beck

(275) In Recognition of the 50th Anniversary of ExxonMobil Corporate Strategic Research: CRE (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Rainbow Spring I/II

Brian M. Weiss, Chair Rajamani Gounder, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 275a: A Personal Historical Perspective of the Last Half Century of Catalysis Researchers at Exxonmobil's Corporate Research Labs

- Stuart L. Soled

8:25 Paper 275b: Understanding Mechanisms in Heterogeneous Catalysis: Fischer-Tropsch and Acid Chemistries Revisited

- Enrique Iglesia

8:50 Paper 275c: The "Dual Challenge" and Natural Gas Conversion Technologies

- David Dankworth

9:15 Paper 275d: Advances in Reaction Design and Engineering for the Production of High Performance Lubricants from Light Olefins

— Suzzy Ho

9:40 Paper **275e**: Zeolites in Industry and Academia – History and Future Perspective

— Avelino Corma

10:05 Paper 275f: Exxonmobil Biofuels Research

- Kelsey McNeely

(276) Materials for Optoelectronic Applications

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 15 Ayaskanta Sahu, Chair Matthew G. Panthani, Co-Chair

Sponsored by: Electronics and Photonics

8:00 Paper 276a: Using Light to Manipulate, Assemble, and Generate Inorganic Nanomaterials in Solution

— Matthew Crane, Elena P. Pandres, E. James Davis, Peter Pauzauskie, Vincent C. Holmberg

8:20 Paper **276b**: From Nanoscale Building Blocks to Functional Fibers — *Vida Jamali*, Farnaz Niroui, Matteo Pasquali, A. Paul Alivisatos

8:35 Paper 276c: Active Plasmonics Based Devices Using Metal Oxide Nanocrystals: Fundamental and Applications

— Ankit Agrawal, Delia J. Milliron

8:50 Paper 276d: Doped Perovskite Nanocrystals for Efficient Blue Light Emitting Diodes

— Daniel Congreve

9:05 Break

9:15 Paper 276e: Controlling Structural Transformations in Sr(Ti,Nb)O₃ Nanocrystals Using Defect Chemistry for Next Generation Ferroelectric Devices

— **Tochukwu Ofoegbuna**, Pragathi Darapaneni, Khashayar R. Bajgiran, Orhan Kizilkaya, James A. Dorman

9:30 Paper 276f: Mid-IR Ag₂se-Based Colloidal Quantum Dot Photodetectors — *Ayaskanta Sahu*, *Dong-Kyun Ko*, *Michael Scimeca*, *Shihab Hafiz*

9:45 Paper 276g: Colloidal CuFeS₂ Nanocrystals: Synthetic Design and Insights into the Unique Optoelectronic Properties Due to Intermediate Fe d-Band

- Sandeep Ghosh, Delia J. Milliron

10:00 Paper 276h: Multi Functional and Multi Color Hybrid Nano-Emitter

— **Tien Hoa Nguyen**, Tiziana Ritacco, Aurélie Broussier, Safi Jradi, Xuan Quyen Dinh, Renaud Bachelot

10:15 Paper **276i**: Exploiting Anti-Stokes Photoluminescence of Quantum Dots to Achieve Optical Cooling

— **Ryan D. Reeves**, Brinkley Artman, Justin J. Hill

(277) Medical Devices I

Tuesday, Nov 12, 8:00 AMHyatt Regency Orlando, Celebration 12/13

Bernard J. Van Wie, Chair Huanan Zhang, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 277a: Rapid Expansion of Cytotoxic T Lymphocytes in a Centrifugal Bioreactor with Applications in Cancer Immunotherapy

— **Kitana Kaiphanliam**, William Davis, Bernard J. Van Wie

8:21 Paper 277b: Enhancing Mass Transfer of Vitamin E to Inflamed Bovine Articular Chondrocytes through Perfusion

— **Haneen Abusharkh**, Olivia Reynolds, Alia Mallah, Mahmoud Amr, Arda Gozen, Juana Mendenhall, Vincent Idone, Nehal I. Abu-Lail, Bernard J. Van Wie

8:42 Paper 277c: A Rapid Convection PCR-Based Diagnostic Platform — *MInGin Kim, Victor M. Ugaz*

9:03 Paper 277d: Digital Single Cell Profiling for Point-of-Care Cancer Diagnosis

— **Jouha Min**, Hyungsoon Im, Hakho Lee, Ralph Weissleder

9:24 Paper 277e: Application of a New Computational Fluid Dynamics Model to Predict Turbulent Flow Damage for the US FDA Critical Path Initiative Centrifugal Blood Pump

— **Mesude Ozturk**, Edgar O'Rear III, Dimitrios V. Papavassiliou **9:45** Paper 277f: Analysis of Pneumonia Associated Volatile Organic Compounds from Bacteria Culture Using Synthesized TiO₂ Nanotube Array Sensor and Gas Chromatography/Mass Spectrometry

— **Yalda Saffary**, Lani McKinnon, Christina Willis, Krista Carlson, Swomitra Mohanty

10:06 Paper **277g:** DNA Recovery from Enteric Bacteria for Rapid Diagnostic Genotyping

— **William G. Pitt**, Ryan L. Wood, Evelyn Welling, Magdalena Crofts, Rebecca Prymak, William C. Beard, Jacob Stepan

(278) Membrane Formation

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Barrel Spring I Yan Wang, Co-Chair Neal Tai-Shung Chung, Co-Chair Hee Jeung Oh, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 278b: Highly Selective MOF Thin-Film Nanocomposite (TFN) Membranes for Water Purification — *Gang Han, Zachary P. Smith*

8:21 Paper 278h: Design of Ultrafiltration (UF), Nanofiltration (NF) and Low-Pressure Reverse Osmosis (LP-RO) Hollow Fiber Membranes for Pressure Retarded Osmosis (PRO) Pretreatment

— Tianshi Yang, Chun Feng Wan, Junying Xiong, Chakravarthy S. Gudipati, **Neal Tai-Shung Chung**

8:42 Paper 278c: Creation of Well-Defined "Mid-Sized" Micropores in Carbon Molecular Sieve Membranes — *Yao Ma*, *Dhaval Bhandari*, *JR Johnson*, *Ryan Lively*

9:03 Paper 278d: Interfacial Hard Templating of Hierarchically Structured, Ultrathin Carbon Molecular Sieve Membranes

— **Megha Sharma**, Mark Snyder

9:24 Paper 278e: Thin-Film Composite Hollow Fiber Membrane with Inorganic Salt Additives for High Mechanical Strength and High Power Density for Pressure-Retarded Osmosis

— **Chun Feng Wan**, Tianshi Yang, Chakravarthy S. Gudipati, Neal Tai-Shung Chung

9:45 Paper **278f**: High Performance Thin Film Composite Membranes with Well-Aligned Nanofiber Substrates for Forward Osmosis Applications

— Chao Han, Xuan Zhang, Yan Wang

10:06 Paper **278g**: Effect of ZIF-8 and Lignin Nanoparticles in Pervaporation Separation of *N*-Butanol from Aqueous Solutions Using PDMS Based Mixed Matrix Membranes

— Ali Zamani**, F. Handan Tezel**, Jules Thibault

(279) Membrane Technology in Food and Bioprocess Engineering

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Celebration 1
Xiaobin Jiang, Chair
Gaohong He, Co-Chair
Chang Dou, Co-Chair

Sponsored by: Food

8:00 Paper 279a: Nanofiltration Process for the Separation of Cephalexin, 7-ADCA and D-Phenylglycine Ternary System — Mengyuan Wu, Xiaobin Jiang, Gaohong He

8:18 Paper **279b**: Combined Osmotic and Membrane Distillation for Concentration of Anthocyaninfrom Muscadine Pomace

— **Arijit Sengupta**, Ranil Wickramasinghe

8:36 Paper **279c**: Comb-Shaped Polybenzimidazole Positively Charged Membranes with Improved Ion Conductivity

— Xuemei Wu, Fujun Cui, Xiaozhou Wang, Shengchun Wu, Gaohong He

8:54 Paper 279d: The Effects of Substrate Morphology on Protein Binding and Elution for Responsive Hydrophobic Interaction Chromatography Applications

— **Shu-Ting Chen**, S. Ranil Wickramasinghe, Xianghong Qian

9:12 Paper 279e: The Vertically Aligned and Opened Carbon Nanotube Filled Polydimethylsiloxane Composite Membrane for Enhanced Butanol Recovery

— **Decai Yang**, Chuang Xue

9:30 Paper 279f: High-Efficient Butanol Production from Non-Detoxified Corn Stover Hydrolysate By Strain Development and Membrane Separation Using Clostridium Acetobutylicum

— Youduo Wu, Chuang Xue

9:48 Paper **279g**: Keynote: Separation of Blood Cells from Plasma through Membranes in Dry Plasma Spot Applications

— **Jie Gao**, Kwee Hiang Jackson Low, Chester L. Drum, E. Shyong Tai, Neal Tai-Shung Chung

(280) Metabolic Engineering: Biosynthetic Pathway Engineering and Enzymatic Conversion for Fine Chemicals

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 3 Mark Blenner, Co-Chair Joshua K. Michener, Co-Chair Han Li, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 280a: Engineering *Yarrowia lipolytica* for the Production of Isoprenoids

— **Georgios Daletos**, Nian Liu, Zhengshan Luo, Zbigniew Lazar, Alkiviadis Chatzivasileiou, Valerie Ward, Jian Chen, Jingwen Zhou, Gregory Stephanopoulos **8:18** Paper 280b: The Isoprenoid Alcohol (IPA) Pathway: A Synthetic Route for Isoprenoid Biosynthesis

— James M. Clomburg, Shuai Qian, Zaigao Tan, Seokjung Cheong, Ramon Gonzalez

8:36 Paper 280c: Enhancing Flavonoid Production By Metabolically Engineered Microbial Co-Cultures

— **Xiaonan Wang**, Lizelle Policarpio, Zhenghong Li, Haoran Zhang

8:54 Paper 280d: Engineering Yeast As the Platform to Characterize and Engineer Biosynthesis of Phytosterols and Derivatives

— Yanran Li

9:12 Paper 280e: Gram-Scale Production of the Psychedelic Natural Product, Psilocybin, in *E. coli*

— Alexandra M. Adams, Nicholas A. Kaplan, John Brinton, Chantal Monnier, Phil O'Dell, Alexis Enacopol, Zhangyue Wei, J. Andrew Jones

9:30 Paper 280f: Genetic Engineering for the Production of Curcuminoids in Mammalian Cells

— Logan Warriner, Daniel W. Pack

9:48 Paper 280g: Engineering Biosynthetic Pathways in Fungi — *Yi Tang*

(281) Metabolic Engineering: Emerging Tools and Technologies

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 2 Kevin V Solomon, Co-Chair Cong T. Trinh, Co-Chair Joshua K. Michener, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 281a: Design of Modular Cells By Goal Attainment Optimization — Sergio Garcia, Cong T. Trinh

8:18 Paper **281b:** Deploying Orthogonal Optogenetic Circuits for Improving Microbial Chemical Production

— **Makoto A. Lalwani**, Evan Zhao, Jose L. Avalos

8:36 Paper 281c: Machine-Leaning and Metabolite Biosensor Assisted Construction of Highly Efficient Saccharomyces Cerevisiae Cell Factory — Yikang Zhou, Xin-Hui Xing, Chong Zhang

8:54 Paper 281d: Building a Comprehensive Set of Genetic Toolkit for Metabolic Engineering of *Issatchenkia Orientalis*

— **Mingfeng Cao**, Vinh Tran, Zia Fatma, Xiaofei Song, Huimin Zhao

9:12 Paper **281e**: Optimization of Pathway Gene Expression from the *Escherichia coli* Chromosome By High-Throughput Screening of Random Site Integration Libraries

— **Tatyana Saleski**, Azzaya Khasbaatar, Meng Ting Chung, Katsuo Kurabayashi, Xiaoxia (Nina) Lin **9:30 Paper 281f:** Resolving Genetic Engineering Signatures in Yeast with the Iseq and Minion on-Site

- Joseph Collins, Eric Young

9:48 Paper 281g: ¹³C-Metabolic Flux Analysis of Microbial Cell Factories for Rational Strain Development

— Yinjie Tang

(282) Micro- and Nano-Scale Technologies in Life Sciences I Tuesday, Nov 12, 8:00 AM

Hyatt Regency Orlando, Celebration 4
Vamsi K. Yadavalli, Co-Chair
Ethan Lippmann, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper 282a: High-Throughput and Scalable Synthesis of Polyanhydride Nanoparticles Via Spray Drying

— **Kathleen Ross, Sean Kelly**, Mellinda Johnston, Balaji Narasimhan

8:18 Paper 282b: Protein— Polyelectrolyte Nanoparticles Via Flash Nanoprecipitation for Enhanced Irreversible Electroporation

— **Shani Levit**, Ross A. Petrella, Christopher C. Fesmire, Michael B. Sano, Christina Tang

8:36 Paper 282c: Utilizing Shape for Selective Targeting of Leukocytes

— Hanieh Safari, Eiji Saito, William Kelley, Lauren Carethers, Lonnie Shea, Omolola Eniola-Adefeso

8:54 Paper 282d: Novel Multicolour Immuno-Labels for Correlative Cathodoluminescence Electron Microscopy

— **Kerda Keevend**, Michael Stiefel, Roman Krummenacher, Egle Truska, Inge K. Herrmann

9:12 Paper 282e: Development of Anti-HER₂ Indocyanine Green-Doxorubicin-Encapsulated Peg-b-PLGA Copolymeric Nanoparticles for Target Photochemotherapy of Breast Cancer Cells *in Vitro*

— Yu-Hsiang Lee, Da-Sheng Chang

9:30 Paper 282f: Integrated Generation of Induced Pluripotent Stem Cells in a Low-Cost Device

— **Ou Wang**, Haishuang Lin, Qiang Li, Qian Du, Leonard Akert, Chi Zhang, Yuguo Leo Lei

9:48 Paper 282g: Invited: A Strawberry-Derived Solution to Oral Protein Delivery

- Kathryn Whitehead

(283) Microreaction Engineering

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom E Kishori T. Deshpande, Chair Andrew R Teixeira, Co-Chair Simon Kuhn, Co-Chair Milad Abolhasani, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 283a: Comparative Study of Indan Oxidation in Microfluidic Reactors

— Yucheng Wu, **Muhammad Siddiquee**, Neda Nazemifard

8:20 Break

8:40 Paper 283c: Design and Scale-up of Biphasic Microreactors for Biomass-Derived Carbohydrates' Conversion

— **Tai-Ying Chen**, Pierre Desir, Mauro Bracconi, Matteo Maestri, Dionisios G. Vlachos

9:00 Paper 283d: Catalytic Mechanism Study of a Palladium-Cyclodextrin Complex for a Suzuki-Miyaura Cross-Coupling with a Microfluidic Reactor

— Yukun Liu, Ryan L. Hartman

9:20 Paper 283e: Design of Multiphase Microreactors Using 3D Printing

— **Yirong Feng**, Haomiao Zhang, Zhengliang Huang, Jingdai Wang, Yongrong Yang

9:40 Paper 283f: Computational Fluid Dynamics Analysis of Microchannel Reactors for Fischer-Tropsch Synthesis: Design Optimization, Thermal Management and Scale-up

— Omar Basha, Nafeezuddin

— **Omar Basha**, Nafeezuddin Mohammad, Shyam Aravamudhan, Debasish Kuila

10:00 Paper 283g: 3D-Printed
Continuous Stirred Tank Mini-Reactor
(CSTmR) for Cell Culture Applications
— Carlos Fernando CeballosGonzález, Salvador Gallegos-Martínez,
Alice Lara-Oriani, Li Lu Lam-Aguilar,
Germán García-Martínez GarcíaMartínez, Christian Carlos MendozaBuenrostro, Juan Felipe Yee-de León,
Ciro Angel Rodríguez-González, Grissel
Trujillo-de Santiago, Mario Moisés
Álvarez

(284) Modeling and Control of Crystallization I

Tuesday, Nov 12, 8:00 AM
Hyatt Regency Orlando, Coral Spring I/II
Zoltan K. Nagy, Chair
Michael Lovette, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00 Welcoming Remarks

8:03 Paper 284a: Crystallization Kinetics of Cephalexin in the Presence of Cephalexin Precursors

— **Matthew A. McDonald**, Andreas S. Bommarius, Martha A. Grover, Ronald W. Rousseau

8:24 Paper 284b: Towards Enhanced Understanding of Sono-Crystallization for Pharmaceuticals

— **Daniel Pohlman**, Moussa Boukerche, Jie Chen, Nandkishor K. Nere

8:45 Paper 284c: Technoeconomic MINLP Optimisation of M.S.M.P.R. Cascades for Continuous Crystallisation of Melitracen Hydrochloride, an Antidepressant API

- Samir Diab, Dimitrios I. Gerogiorgis

- 9:06 Paper 284d: Controlled Manipulation of the Size and Shape of Needle-like Crystals in a Cyclic Process - Stefan Boetschi**, Ashwin Kumar** Rajagopalan, Manfred Morari, Marco Mazzotti
- 9:27 Paper 284e: Digital Design and Operation of Continuous Crystallization Processes Via Mechanistic Modelling - Niall Mitchell, John Mack, Furgan Tahir, Cameron Brown, Tariq Islam, John Robertson, Eduardo Lopez-Montero, Alastair J. Florence
- 9:48 Paper 284f: Quality By Control (QbC) Guided Quality By Design (QbD) for the Optimal Operation of Integrated Crystallizer-Wet Mill Systems
- Botond Szilagyi, Zoltan K. Nagy

(285) Multiscale Systems Biology Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 14 Ashlee N. Ford Versypt, Chair Mark P. Styczynski, Co-Chair Steven M. Abel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- 8:00 Paper 285a: Quantifying the Impact of Cellular Heterogeneity on CGAS Pathway Regulation Using Multiscale Agent-Based Modeling — **Robert W. Gregg**, Jason E. Shoemaker
- 8:18 Paper 285b: Intercellular Biochemical Cross-Talk at the Onset of Diabetic Kidney Disease
- Minu R. Pilvankar, Ashlea D. Sartin, Claire Streeter, Steve M. Ruggiero, Ashlee N. Ford Versypt
- 8:36 Paper 285c: To Bundle or Not. Morphological Transitions in Actin Bundles Are Determined By Their Initial Polarity, Myosin Activity, Crosslinking, and Filament Treadmilling
- Aravind Chandrasekaran, Garegin Papoian, Arpita Upadhyaya
- 8:54 Paper 285d: Quantitative, Multi-Scale Modeling Using Qualitative Data Identifies a Plant-Specific Dual Role for Hops in Regulated Vacuole Fusion
- Belinda S. Akpa, David Flaherty, Aniket Antad, Natalie Clark, Rosangela Sozzani, Marcela Rojas-Pierce
- 9:12 Paper 285e: Multiscale Multiobjective Systems Analysis (MIMOSA): An Advanced Metabolic Modeling Framework for Complex Systems
- Joseph Gardner, Bri-Mathias S. Hodge, Nanette R. Boyle
- 9:30 Paper 285f: Metabolic Modeling of Sphingolipid Metabolism to Elucidate the Flux Changes and Regulatory Events Induced By Biologically-Significant Perturbations
- **Adil Alsiyabi**, Rajib Saha
- 9:48 Paper 285g: Invited: Bridging from Protein-to-Tissue with Multiscale Computational Models
- Shayn Peirce-Cottler

(286) Oxygen and Hydrogen Photocatalysis and Electrocatalysis I

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Florida Ballroom A Elizabeth J. Biddinger, Chair

Linsey Seitz, Co-Chair

Sponsored by: Catalysis and Reaction **Engineering Division**

- 8:00 Paper 286a: Quantifying Kinetic Barriers in Alkaline Hydrogen Electrocatalysis through Single-Crystal Voltammetry and Kinetic Isotope Effects - Luis Rebollar, Saad Intikhab, Joshua Snyder, Maureen H. Tang
- 8:18 Paper 286b: pH, Cation, and Ad-Atom Effects on Hydrogen Oxidation and Evolution Reaction Kinetics
- lan T. McCrum, Marc T.M. Koper
- 8:36 Paper 286c: Nife Alloy Nanotube Arrays As Highly Efficient Bifunctional Electrocatalysts for Overall Water Splitting at High Current Densities
- Chun-Lung Huang, Xui-Fang Chuah, Cheng-Ting Hsieh, Shih-Yuan
- 8:54 Paper 286d: Selective Silicon Oxide Overlayers for Sustainable Hydrogen Production By Seawater Electrolysis
- Amar A. Bhardwaj, Daniel V. Esposito, Ngai Yin Yip
- 9:12 Paper 286e: Understanding Pt's Unique Activity in Hydrogen Evolution - Andrew A. Peterson, Per Lindgren, Geora Kastlunger
- 9:30 Paper 286f: Structural Analysis of Chalcogenide-Functionalized Precious Metal Nanoparticles from First Principles - Jeffrey S. Lowe, Vamakshi Yadav, Alexander J. Shumski, Christina W. Li,
- 9:48 Paper 286g: Electrochemical Stability and Hydrogen Evolution Activity of Bare and Platinum-Modified Tungsten and Niobium Nitrides

Jeffrey Greeley

- Steven R. Denny. Brian M. Tackett. Dong Tian, Qian Zhang, Kotaro Sasaki, Jingguang G. Chen
- 10:06 Paper 286h: Electrocatalytic and Optoelectronic Characteristics of Exfoliated Two-Dimensional Titanium Nitride Ti, N, Tx mxene
- Abdoulaye Djire, Hanyu Zhang, Jun Liu, Elisa Miller, Nathan Neale

(287) PAT and Process Monitoring in Crystallization Development and Manufacturing

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Manatee Spring I Ben Yang, Chair Sohrab Rohani, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00 Welcoming Remarks

- 8:03 Paper 287a: Model Based Optimization of Cooling Crystallization of Active Pharmaceutical Ingredients **Undergoing Thermal Degradation** - Kanjakha Pal, Zoltan K. Nagy
- 8:24 Paper 287b: Resolution By Crystallization: The Quest for Chiral Purity
- Andrew Byrne, Mark Barrett, Brian
- 8:45 Paper 287c: Reactive Agglomeration: Improving Processability of Amorphous Solids in Precipitation
- Sandeep Ippalapalli, Amol Ashok Pawar, Suhas Jawlekar, Srividya Ramakrishnan
- 9:06 Paper 287d: Surprisingly Complex Phase Behavior of 3,5,5-Trimethylpyrrolidin-2-One Affecting Its Chiral Puirty Enrichment through Crystallization — Jicong Li
- 9:27 Paper 287e: Mechanistic Investigation of Spherical Crystallization of Active Pharmaceutical Ingredients Using in-Situ PAT and Mathematical Models
- Kanjakha Pal, Zoltan K. Nagy
- 9:48 Paper 287f: Continuous Crystallization of Carbamazepine in Oscillatory Baffled Crystallizer
- Jiaxiang Zhang, Xiaochuan Yang, David A. Acevedo, Sean Naimi, Jiahao Wu, Sonal Mazumder, Celia N. Cruz, Thomas O'Connor
- 10:09 Paper 287g: Kinetic Assessment for Continuous Crystallization Process Development of an Early Development Compound
- Gladys Kate Pascual, Marko Ukrainczyk, Gary Morris, Brian Glennon, Alain Collas, Ronny Vanierschot

(288) Plenary Session: **Chromatographic Separations** and SMB - In Honor of Linda Wang (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Manatee Spring II Arvind Rajendran, Chair

Sponsored by: Adsorption and Ion

- 8:00 Paper 288a: Professor Linda Wang's Research Group - the Early Years
- Roger D. Whitley
- 8:20 Paper 288b: Simulated Moving Bed- Learning from the Past and Shaping the Future
- Alírio E. Rodrigues, Jonathan Gonçalves
- 8:40 Paper 288c: Potential Roles of a Simulate-Moving-Bed Chromatography As a Final-Step Purification Process for the Production of High-Valued Products from Marine Algae Biomasses
- Sungyong Mun

- 9:00 Paper 288d: Design of Bypass-Simulated Moving Bed Process for Reduced Purity Requirements - Rafael Terruo Maruyama, Preetika Karnal, Tuomo Sainio, Arvind Rajendran
- 9:20 Paper 288e: The Rigid Adsorbent Lattice Fluid Model Applied to the Correlation of Liquid Phase Partition Coefficients of Different Solvents in MFI Zeolites
- Roberto Mennitto, Lev Sarkisov, Stefano Brandani
- 9:40 Paper 288f: Improving Indoor Air Quality: Determining Adsorption Properties of VOC's Using Concentration Pulse Chromatography
- Ji Sub Yun, Sean Wilson, F. Handan Tezel
- 10:00 Paper 288g: Upgrading of Low-Value Carbon Precursors to Porous Carbon Materials for Greenhouse Gas Capture
- Ki Bong Lee
- 10:20 Concluding Remarks by Prof. Linda Wang

(289) Polymer Networks, Gels, and **Crosslinked Systems I**

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 11 Santanu Kundu, Chair Nese Orbey, Co-Chair

Sponsored by: Polymers

- 8:00 Paper 289a: Associative Gels with Crystalline and Semicrystalline Domains: Softer Junctions Can Yield Stiffer Gels
- Xuechen Yin, David Hewitt, Robert B. Grubbs**, Surita Bhatia**
- 8:15 Paper 289b: Mussel-Inspired, Tough Elastomer with Dynamic Bonding Ameya Narkar, Kollbe Ahn
- 8:30 Paper 289c: Mechanical Phase Transitions and Elastic Anomalies in Biopolymer Gels
- F.C. MacKintosh
- 9:00 Paper 289d: Molecular Anisotropy and Rearrangement As Mechanisms of Toughness and Extensibility in Entangled Physical Gels - Chelsea E. R. Edwards, Danielle J. Mai, Shengchang Tang, Bradley D. Olsen
- 9:15 Paper 289e: Programming Deformation in Liquid Crystalline
- Timothy White, Hayden Fowler, Anesia Auguste
- 9:30 Paper 289f: Structure and Dynamics of Polyelectrolyte Complex Hydrogels
 - Defu Li, Samanvaya Srivastava
- 9:45 Paper 289g: Structural Guides: Influence of High Molecular Weight Polymer Additives on Low Molecular Weight Gels Towards Solid-State, Composites
- LaShanda T.J. Korley, Symone Alexander

10:00 Paper 289h: Controlled Release of Insect Repellent from Biopolymer Core-Shell and Matrix Microcapsules — James Ogilvie-Battersby, Rashmi Sharma, Nese Orbey, Ramaswamy Nagarajan, Jayant Kumar, Ravi Mosurkal

10:15 Paper 289i: Rational Design of Tissue-like Materials with Hydrogel Systems Embedding Granule Particles and Soft Liquid Metal Nanoparticles

— Yiliang Lin, Yin Fang, Bozhi Tian

(290) Process Intensification and Modular Manufacturing: Modular/Advanced Manufacturing

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 28 Paul Yelvington, Chair Fereshteh Farzad, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

- **8:00** Paper 290a: A Case Study for the Use of Conventional and Modular Construction Methods in Building an Intensified Chemical Plant
- **Brian K. Paul**, James O'Connor, Karl Haapala, Arvind Shankar Raman, Khaled Alhamouri
- **8:25** Paper **290b**: Modular Ethane-to-Liquids Via Low-Temperature Chemical Looping Oxidative Dehydrogenation of Ethane
- **Luke Neal**, Vasudev Pralhad Haribal, Fanxing Li
- **8:50 Paper 290c:** On Demand Treatment of Wastewater Using 3D-Prined Membrane
- **Corey Clifford**, Bingchen Wang, Aigerim Baimoldina, Yihan Song, Tao Hung, Cliff Kowall, Lei Li
- **9:15** Paper **290d:** Selecting Membrane Distillation Configuration *M. R. Islam, Chau-Chyun Chen*,
- M. R. Islam, Chau-Chyun Chen, Mahdi Malmali
- **9:40 Paper 290e:** Deploying Intensified, Automated, Mobile, Operable, and Novel Designs "Diamond" for Treating Shale Gas Wastewater
- **Debalina Sengupta**, Joseph Sang-Il Kwon, Phil Carlberg, Lucy Mar Camacho, Joan F. Brennecke, Mark Stadtherr, Benny D. Freeman, Vikas Khanna, Radisav Vidic, Mahmoud El-Halwaqi

(291) Reaction Path Analysis Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom F Heather Mayes, Chair Xinrui Yu, Co-Chair Prasanna Dasari, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 291a: First-Principles Kinetic Monte Carlo Study of Biomass Conversion over Ru/TiO₂

— **Xiao Li**, Lars C. Grabow

- **8:18** Paper 291b: Reaction Paths Predicted for Xylose and Xylan Pyrolysis Chemistry Using Reactive Molecular Dynamics
- **Gayathri Janarthanam**, Amrutha Raghu, Phillip R. Westmoreland
- **8:36 Paper 291c:** Elucidating Additive Effects on Oligomerization Reaction Mechanisms during Solid-Electrolyte Interphase Formation Using Molecular Simulations
- Luke D. Gibson, Jim Pfaendtner
- **8:54 Paper 291d:** Elucidation of the Mechanism for Ethene Hydrogenation over Single Metal Cation Catalysts: A Combined Modeling and Experimental Study
- **Hafeera Shabbir**, Steven Pellizzeri, Magali Ferrandon, In Soo Kim, Massimiliano Delferro, Alex Martinson, Rachel B. Getman
- **9:12** Paper **291e:** Sampling Time-Resolved Reaction Pathways for Chemical and Biochemical Reactions in Solvent and in Enzyme
- **Zhongyue Yang**, Charles Doubleday, Kendall Houk
- **9:30 Paper 291f:** How Basic Sites Strength Influences the Guerbet Reaction
- **Giada Innocenti**, Juliana Velasquez Ochoa, Alessandro Ponti, Massimo Mella, Fabrizio Cavani
- **9:48 Paper 291g:** Solvent Reaction Coordinate for an SN₂ Reaction
- **Christian Leitold**, Marcel D. Baer, Christopher J. Mundy, Gregory Schenter, Baron Peters
- **10:06 Paper 291h:** Top-Down Kinetic Modeling: A Transient Solution Strategy to Assess Benzene Hydrogenation Kinetics
- **Ana R. Costa da Cruz**, Jeroen Poissonnier, Ana Obradović, Kenneth Toch, Joris W. Thybaut

(292) Special Session: Celebrating Career Accomplishments of Fred Zenz

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 19 Reddy Karri, Chair

Sponsored by: Fluidization and Fluid-Particle Systems

- **8:00 Paper 292a:** What Is Happening Above Your Fluidized Beds?
- **Reddy Karri**, Ben Freireich, Ray Cocco
- **8:25** Paper 292b: The Origins and Evolution Of Cyclone Design: How Innovation and Miss-steps Led To The Current State Of Cyclone Design *Jonathon Zenz*
- **8:50** Paper **292c:** Career Long Work On Bulk Solids Handling Projects *Thomas F. McGowan*
- 9:15 Paper 292d: Cyclones a la Zenz?

 T. M. Knowlton, Reddy Karri
- **9:40** Paper 292e: Fred Zenz A Graduate Student Perspective? *Roy Silverman*

(293) Technologies for Understanding Microbial Interactions Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Celebration 9 Connie B. Chang, Chair

Sponsored by: Microbes at Biomedical Interfaces

Jing Yan, Co-Chair

- **8:00 Paper 293a:** Invited Speaker: Understanding Virus Surface Interactions and Stability
- Caryn L. Heldt, Xue Mi, Whitney C. Blocher McTigue, Mallory Bunker, Pratik U. Joshi, Sarah L. Perry
- **8:18** Paper 293b: Preventing Bacterial Biofilm Formation Using Active Surface Topography
- **Huan Gu**, Sang Lee, Dacheng Ren
- **8:36** Paper 293c: Invited Speaker: Developing Tools to Study and Engineer Microbes Beneficial to Human Health *Nikhil U. Nair*
- **8:54** Paper 293d: Invited Speaker: Developing and Applying a Microdroplet Co-Cultivation and Omics Toolbox for Elucidating Microbiomes
- Xiaoxia Nina Lin
- 9:12 Paper 293e: Microsphere Hydrogel Encapsulation to Identify Interactions in Chronic Wound Microbial Consortia
- **Shawna Pratt**, Petria Russell, Connie B. Chang
- 9:30 Paper 293f: Invited Speaker: Drop Stabilization on a Chip (DropSOAC): Stabilizing Microfluidic Drops for Time-Lapse Quantification of Single-Cell Bacterial Physiology
- Connie B. Chang
- **9:48** Paper 293g: Invited Speaker: Designing Functional Nanoculture Systems for Studying Microbial Dynamics
- Tagbo H.R Niepa, Huda Usman
- 10:06 Paper 293h: Invited Speaker: Efforts Toward Measurement Assurance for Microbial Biofilm Characterization — Nancy J. Lin, Sandra M. Da Silva, Kirsten Parratt, Joy Dunkers

(294) The Energy-Water Nexus Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Regency Ballroom V Shweta Singh, Chair Jason Trembly, Co-Chair Urmila M. Diwekar, Co-Chair

Sponsored by: Sustainable Energy

- **8:00 Paper 294a:** Evaluating Energy-Water Nexus Tradeoffs for U.S Rice Production
- **Nemi Vora**, Colin P Gillen, Oleg A Prokopyev, Vikas Khanna
- **8:25** Paper 294b: Cooling Tower Design for the Water – Energy Nexus: Effect of Weather Conditions on Water Consumption and Tower Sizing
- Lidia S. Guerras, Mariano Martín

- **8:50** Paper **294c:** Scenario Reduction for Power System Planning and Scheduling Problems Under Energy-Water Nexus Considerations

 R. Cory Allen, Styliani Avraamidou, Efstratios N. Pistikopoulos
- **9:15** Paper 294d: Modeling and Techno-Economic Optimization of Desaliantion Technologies for Produced Water Treatment
- **Elmira Mohammadi Shamlou**, Radisav Vidic, Vikas Khanna
- **9:40 Paper 294e:** Using Solar Powered Mixing Devices to Reduce Dissolved Iron in a Drinking Water Reservoir
- Jason A. Heberling

(295) Tools and Techniques for Product Design

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 17 Duygu Gerceker, Chair Anand N. Vennavelli, Co-Chair Shaibal Roy, Co-Chair

Sponsored by: Product Design

- **8:00** Paper 295a: Group Contribution Method for Organosilicon Compounds *Yijia Sun, Nick Sahinidis*
- **8:25 Paper 295b:** Molecular Simulations for the Design and Property Prediction of Elastomer Seals for Sour Gas Environments
- **Sitaraman Krishnan**, Miao Luo, Zackary A. Putnam
- 8:50 Paper 295c: Formulation of Post Cobalt CMP Cleaning Solution Based on Stability Constants of Metal Complexes S. S. R. K. Hanup Vegi, J. Seo, C.K. Ranaweera, N. K. Baradanahalli, S. V. Brahu
- **9:15** Paper **295d:** Multi-Scale Approach to Evaluate Emulsification Variables (Tip Velocity and Pumping Capacity) on Texture, Rheology and Stability of O/W Cosmetic Emulsions
- **Fernando Calvo**, Jorge M. Gómez, Oscar A. Alvarez
- **9:40 Paper 295e:** Procapd: A Smart Tool for Computer-Aided Chemical Product Design
- **Lei Zhang**, Haitao Mao, Anjan Kumar Tula, Mario Richard Eden, Rafiqul Gani
- **10:05** Paper **295f**: Digitalization to Drive Differentiation in a Hyper-Competitive Plastics Industry

 Narayan Ramesh

(296) Turbulent and Reactive Flows and Flow Characterization

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom M Nicolas J. Alvarez, Co-Chair

Cari S. Dutcher, Co-Chair

Sponsored by: Fluid Mechanics

- 8:00 Paper 296a: Flow Visualization of the Horizontal Tube Reactor with an Open Outlet
- Taeseon Lee, Taewoong Um, Jinhwan Park, In Seok Kang**, Kun-Hong**
- 8:15 Paper 296b: Curvature Dependence of Viscoelastic Turbulent **Taylor-Couette Flows**
- Bamin Khomami, Nansheng Liu, Jiaxing Song, Hao Teng, Xiyun Lu, Hang Ding
- 8:30 Paper 296c: Taylor-Couette Flow Behavior with Polyelectrolyte Solutions - Athena E. Metaxas, Vishal Panwar, Cari S. Dutcher
- 8:45 Paper 296d: Spatially Invariant K-Means Clustering for Analyzing the Turbulent Attractor of Minimal Channel Flow
- Alec Linot, Michael D. Graham
- 9:00 Paper 296e: The Influence of Chemical Reactions on Turbulent Mixing - Charles A. Petty, André Bénard
- 9:15 Paper 296f: Drag Reduction and Degradation of Diutan Biopolymer Solutions during Turbulent Flow in a 4.6 Mm ID x 200 L/D Smooth Pipe - Preetinder S. Virk
- 9:30 Paper 296g: Helicity in Turbulent Transport
- Dimitrios V. Papavassiliou, Quoc T. Nguyen
- **9:45** Break
- 10:00 Paper 296i: Effects of Light Gas Addition on Biomass Pyrolysis in **Bubbling Fluidized Beds**
- Zachary Mills, Gavin Wiggins, Xi Gao, Charles E. A. Finney, Bruce Adkins, Jim Parks

(297) Tutorial Session on **Electrochemical Methods, Systems** and Applications (Invited Talks)

Tuesday, Nov 12, 8:00 AM Hvatt Regency Orlando, Plaza International Ballroom I **Daniel Esposito, Chair** John Harb, Co-Chair Thomas F. Fuller, Co-Chair Robert J. Messinger, Co-Chair

Sponsored by: Electrochemical Fundamentals

- 8:00 Paper 297a: Breakthrough Electrolytes for Energy Storage (BEES) Robert F. Savinell
- 8:35 Paper 297b: Electronic Structure Modeling of Electrocatalysis at the Electrode-Electrolyte Interface — Michael J. Janik
- 9:10 Paper 297c: Tutorial on Electrodeposition and the Rotating Hull Cell
- Elizabeth J. Podlaha
- 9:45 Paper 297d: Systematic Model **Development for Electrochemical** Impedance Spectroscopy
- Mark E. Orazem

(298) Value-Added Chemicals from **Natural Gas**

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Challenger

Dushyant Shekhawat, Chair Götz Veser, Co-Chair Jianli Hu, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

- 8:00 Paper 298a: Copper Speciation in Cu-Mordenite Catalysts for the Oxidation of Methane to Methanol
- Gordon Brezicki, James D. Kammert, Yuanging Wang, Jutta Kröhnert, Chris Paolucci, T. Brent Gunnoe, Annette Trunschke, Robert Schlögl, Robert J. Davis
- 8:18 Paper 298b: Dual Production of Higher Hydrocarbons and Syngas from Greenhouse Gases in a Hydrogen-Permeable Membrane Reactor
- Mann Sakbodin, Eric D. Wachsman, Donaxia Liu
- 8:36 Paper 298c: Elucidating the interactions of H₂S and CO₂ with transition metal sulfide catalysts for natural gas upgrading
- Lohit Sharma, Ronak Upadhyay, Srinivas Rangarajan, Jonas Baltrusaitis
- 8:54 Paper 298d: Understanding the Synergistic Effects of Feed Composition and Metal Oxide Formulation in a Chemical Looping Oxidative Coupling of Methane System
- Deven Baser, Zhuo Cheng, Lang Qin, Liang-Shih Fan
- 9:12 Paper 298e: Mo Oxide Supported on Sulfated Hafnia: Novel Catalyst for Activation of Propane
- Ashraf Abedin, Swarom Kanitkar, Srikar Bhattar, James J. Spivey
- 9:30 Paper 298f: Nanographene By Microwave-Assisted Plasma-Mediated Methane Pyrolysis: Spectroscopic and Microscopic Characterization
- Raiu Kumal, Akshav Gharpure. Randy Vander Wal, Kurt Zeller, Aayush Mantri, George Skoptsov
- 9:48 Paper 298g: Low-Thermal-Budget Conversion of Natural Gas Integrated with Industrial Electrification
- **Dong Ding**, Wei Wu, Lu-Cun Wang
- 10:06 Paper 298h: Transforming Living Methanotrophs into Chemical Reactors — **Jennifer M. Knipe**, Samantha Ruelas, Hawi Gemeda, Joshua R. Deotte, Joshuah Stolaroff, Sarah E. Baker, Calvin Henard, Michael Guarnieri,

(299) What to Expect Moving from **Graduate School to Your Future** Tuesday, Nov 12, 8:00 AM

Hyatt Regency Orlando, Bayhill 32 Cory Thomas, Co-Chair

Sponsored by: Young Professionals Committee (YPC)

(300) Woman Chemical Engineers: **Managing to Retain Them**

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Bayhill 18 Quinta Nwanosike Warren, Chair **Donna Bryant, Co-Chair**

Sponsored by: Management Division

- 8:00 Welcoming Remarks
- 8:05 Paper 300a: Background and Discussion about Retaining Women Engineers
- Urmila M. Diwekar
- 8:20 Paper 300b: Background and Discussion about Retaining Chemical **Engineering Women in Industry** - Gayle Gibson
- 8:35 Paper 300c: Background and Discussion about Retaining Women in
- Ana Davis
- 8:50 Panel Discussion
- 9:35 Concluding Remarks

(301) Area Plenary: Carbon Nanomaterials (Invited Talks)

Tuesday, Nov 12, 8:30 AM Hyatt Regency Orlando, Discovery 44 Geyou Ao, Chair Anson Ma, Co-Chair

Sponsored by: Carbon Nanomaterials

- 8:30 Paper 301a: Controlled Functionalization of Carbon Nanomaterials for Multifunctional Applications
- -Liming Dai
- 9:30 Paper 301b: Carbon Nanomaterial Dispersions Grow up - 18 Years of Adventures of Probing Dispersion State to Improve Final **Properties**
- Virginia Davis

(302) Ammonia Synthesis: Next Generation Technology I

Tuesday, Nov 12, 10:20 AM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

- 10:20 Paper 238c: Sustainable Ammonia Production from Sun, Air and
- Dorottya Guban, Josua Vieten, Martin Roeb, Christian Sattler
- 11:06 Paper 302b: Optimizing Absorptive Separation for Intensification of Ammonia Production
- Mahdi Malmali
- 11:29 Paper 302c: 300°C Proton-**Exchange Membrane for Low-Pressure** Electrolytic Ammonia Synthesis **Ted Aulich**
- 11:52 Paper 302d: Microwave Catalytic Synthesis of Ammonia for Energy Storage and Transformation
- Xinwei Bai, Dushyant Shekhawat, Christina Wildfire, Albert E. Stiegman, Robert A. Dagle, Jianli Hu

- 12:15 Paper 302e: Energy Storage through Electrochemical Ammonia Synthesis Using Proton-Conducting Ceramics
- Neal P. Sullivan, Liangzhu Zhu, Chuancheng Duan, Ryan O'Hayre, Max Pisciotta, Long Le, Carolina Herradon Hernandez, Michelle Butler, Canan Karakaya, Robert J. Kee, Fred Jahnke, Hossein Ghezel-Ayagh

(303) MAC/MFF Real Talk: Navigating the Academic Career Path to Tenure (Ticketed Event)

Tuesday, Nov 12, 11:00 AM Hyatt Regency Orlando, Gulf Reginald E. Rogers Jr., Chair Gilda Barabino, Co-Chair

Sponsored by: Minority Affairs Committee (MAC)

(304) Meet the Innovators: Transforming the Future through Chemical Engineering (Invited Talks)

Tuesday, Nov 12, 11:00 AM Hyatt Regency Orlando, Plaza International Ballroom G Venkat R. Bhethanabotla, Chair Richard Dickinson, Co-Chair

Sponsored by: Liaison Functions

- 11:00 Paper 304a: Chemical Engineering Innovations for a Renewable Economy Rakesh Agrawal
- 11:20 Paper 304b: Innovations in Synthetic Biology - Jay D. Keasling
- 11:40 Paper 304c: Engineering Materials for Clinical Application **Christine Schmidt**
- 12:00 Panel Discussion

(305) Andreas Acrivos Award for **Professional Progress in Chemical Engineering Lecture**

Tuesday, Nov 12, 11:15 AM Hyatt Regency Orlando, Plaza International Ballroom H Orlin D. Velev, Chair

Sponsored by: Awards Committee

11:15 Paper 305a: Control of Interfacial Stability in Electrochemical Systems - Martin Z. Bazant

(306) Advances in Biosensors and **Biodiagnostics: Systems and Devices** for Advanced Biosensing

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 3 Hyun J. Kwon, Co-Chair Stephanie McCalla, Co-Chair Chang Liu, Co-Chair Xiao-an Fu, Co-Chair Kevin J. Cash, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 306a: Sequence-Specific Nucleic Acid Detection at <1 Am — Harold G. Monbouquette

12:48 Paper 306b: Detection of Water-Borne Pathogens Using a Smartphone-Based Portable Isothermal Amplification Platform

- Aashish Priye

- **1:06** Paper 306c: Cell Tracking Velocimetry: A Femtogram Resolution Fluorescence Cytometric Magnetometer — *James Kim, Jeffrey Chalmers*
- **1:24** Paper 306d: On-chip bio-sensor for microbial contamination

 Bharat Maddipudi, Hope Dosch,
- Vinod S. Amar, Anuradha Shende, Rajesh Shende
- **1:42** Paper 306e: Malaria Smartphone Diagnostic Using Isothermal Amplification
- **Ashlee Colbert**, Katherine N. Clayton, Jacqueline Linnes, Tamara L. Kinzer-Ursem
- **2:00** Paper 306f: Hollow Fiber Microfiltration Principles Impacting Pathogen Recovery to Enable Rapid Detection
- **Jessica Zuponcic**, Casey Bomrad, Jorge N. Velez, Kirk Foster, Eduardo Ximenes, Michael R. Ladisch
- **2:18** Paper 306g: Invited Speaker Biosensor Systems and Devices *Kevin J. Cash*

(307) Advances in Cell Culture Engineering and Biopharmaceutical Manufacturing

Tuesday, Nov 12, 12:30 PM
Hyatt Regency Orlando, Celebration 14
Amit Kumar Jha, Chair
Clayton S Jeffryes, Co-Chair
Xiao-an Fu, Co-Chair
Nikhil U. Nair, Co-Chair
Yong-Chan Kwon, Co-Chair
Aravindan Rajendran, Co-Chair

Sponsored by: Bioengineering

- **12:30** Paper **307a**: Application of a High Throughput Workflow from FIH Process Development to PC for Therapeutic Proteins
- **Cameron Phillips**, Niket Bubna, David Chang, Sigma Mostafa, Derek Rvan
- **12:48** Paper 307b: Block Co-Polymer $P_{\rm 188}$ Contributes to Increased Viability and Harvest Duration for High Density Perfusion Cell Culture
- Peter Amaya
- **1:06** Paper 307c: High Titer Production of Plasmid DNA in Disposable Fermentors
- **Mark Berge**, Rohan Patel, Shushil Machhi
- **1:24** Paper 307d: Improving Platform Process Feeding Strategy Using an lvcc-Based Approach for CHO-M Cell Lines
- **Jake Kim**, Niket Bubna, Sigma Mostafa, James Hamlin, Dane Grismer
- 1:42 Paper 307e: Prediction and Experimental Validation of Oxygen Transfer in a Rocking Disposable Bioreactor
- **Yun Bai**, William Anderson, Murray Moo-Young

- **2:00** Paper 307f: On the impact of Nutrient Supplementation Strategies on antibody producing CHO cell cultures *Ricardo Suarez Heredia*,
- Alexandros Kiparissides

 2:18 Paper 307g: Boosting the
 Activity of CHO-Based Cell-Free Protein
- Activity of CHO-Based Cell-Free Protein Synthesis Factories for High-Throughput in Vitro Production of Functional Antibodies
- **Chiara Heide**, Gizem Buldum, Oscar Ces, Cleo Kontoravdi, Karen Polizzi

(308) Advances in Methane Coupling Reaction and Aromatization

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Challenger 41/42

Dushyant Shekhawat, Chair Jianli Hu, Co-Chair Götz Veser, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

- 12:30 Paper 308a: Techno-Economic Analysis of Direct Methane Aromatization for Natural Gas Upgrading with Mini-Plant Construction for Remote Deployment
- **Michael Sees**, Lauren Ward, Chau-Chyun Chen, Sheima J. Khatib
- **12:48 Paper 308b:** Non-Oxidative Methane Conversion: Coupling Gas-Phase and Surface Models of Fe Single-Site Catalysts
- **Jongyoon Bae**, Javad Hashemi, C. Franklin Goldsmith, Andrew A. Peterson
- **1:06 Paper 308c:** Catalyst Design for Microwave Assisted Methane Dehydroaromatization
- Yifan Deng, Sanjana Karpe, Victor Abdelsayed, Dushyant Shekhawat, Jianli Hu, Götz Veser
- 1:24 Paper 308d: Microwave Assisted Catalytic Conversion of Ethane to Aromatics for a More Efficient Approach over a Conventional Fixed Bed Reactor Brandon Robinson, Ashley Caiola, Xinwei Bai, Jianli Hu
- 1:42 Paper 308e: Effects of Low Dopant Concentrations on the Performance of Samarium Oxide in the Oxidative Coupling of Methane
- **Andrew S Jones**, Helena Hagelin-Weaver, Marcus Bäumer, Jan Ilsemann
- 2:00 Paper 308f: Enhancing Selectivity in Oxidative Coupling of Methane Using Catalytic Solid Oxide Membrane Reacting Systems
- **Valentina Omoze Igenegbai**, Randall Meyer, Suljo Linic
- 2:18 Paper 308g: Multi-Scale Simulation Framework for the Oxidative Coupling of Methane: From Process Layouts to Catalyst Particles
- Laura Pirro, Pedro S.F. Mendes, Bram Kemseke, Bart D. Vandegehuchte, Guy B. Marin, Joris W. Thybaut

- 2:36 Paper 308h: Single Site
 Vs Crystalline: Development and
 Characterization of Mn/W/Na/SiO₂ Model
 Catalysts for the Oxidative Coupling of
 Methane (OCM)
- Daniyal Kiani, Sagar Sourav, Jonas Baltrusaitis, **Israel E. Wachs**

(309) Advances in Nuclear and Hazardous Waste Processing and Disposal

Tuesday, Nov 12, 12:30 PM
Hyatt Regency Orlando, Discovery 43
Thong Hang, Chair
Dan P. Lambert, Co-Chair
Robert W. Peters, Co-Chair

Sponsored by: Nuclear Engineering Division

- 12:30 Paper 309a: Evaluation of Chemical Additives for Glycolate Destruction in High-Level Radioactive Waste Condensate in the Defense Waste Processing Facility
- Dan P. Lambert
- **12:51** Paper 309b: Tank Closure Cesium Removal at Savannah River Site — *Terri Fellinger, Aubrey I. Silker, Mark Keefer*
- 1:12 Paper 309c: Large Cemented Gibbsite Agglomerates in Alkaline Nuclear Waste at the Hanford Site and the Impacts to Remediation
- **Jacob Reynolds**, Jason Page, Gary Cooke, Beric Wells
- **1:33** Paper 309d: Processing of Actinide Materials for Reuse/Disposal *Sharon Robinson*, *Brad Patton*
- 1:54 Paper 309e: In-Situ Raman and ATR-FTIR Spectroscopy for Monitoring of Molecular Species in Low-Activity Nuclear Waste
- **Stefani Kocevska**, Giovanni Maria Maggioni, Martha A. Grover, Ronald W. Rousseau
- 2:15 Paper 309f: Ultra-Microporous Materials for Efficient Removal of Krypton from Nuclear Reprocessing Facilities
- **Sameh Elsaidi**, Mona Mohamed, David Hopkinson, Ahmed Helal, Ju Li, Praveen K. Thallapally
- **2:36** Paper 309g: The Migration Law of Nuclides in Steam Reforming Reaction of Spent Radioactive Resins
- **Qi Song**, Yao Yang, Jingyuan Sun, Zhengliang Huang, Jingdai Wang, Yongrong Yang

(310) AIChE Management Award Recipient Presentation Session: Focusing on Technology and Innovation Management

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Florida Ballroom C

Joseph J. Cramer, Chair George Newcomb, Co-Chair

Sponsored by: Management Division

- **12:30** Paper **310a**: My Management Journey, from Technology Developer to Innovation Leader
- Cristina Thomas
- 1:15 Paper 310b: Impacts on Management from an Evolving World and Profession
- Phillip R. Westmoreland
- **1:45 Paper 310c:** Advancing Technology Though Measurement Science
- Eric Lin
- **2:15** Paper 310d: Engineering and Science at the National Laboratories *Juan J. DePablo*
- **2:45 Paper 310e:** General Question and Answer Period
- **Joseph J. Cramer**, George Newcomb

(311) Applications in Immunology and Immunotherapy

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 2 Roger Harrison, Chair Jason E. Shoemaker, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- 12:30 Paper 311a: Controlling Cellular Phenotypes Via Cytokine-Releasing Backpacks for Cancer Immunotherapy C. Wyatt Shields IV, Michael A Evans, Li-Wen Wang, Siddharth Iyer, Debra Wu, Anusha Pusuluri, Samir Mitragotri
- **12:48** Paper **311b:** Enhancing the Tumor Selectivity of Targeted Proteins through Avidity Optimization *Clifford M. Csizmar, Jacob R. Petersburg, Lakmal Rozumalski,*

Benjamin J. Hackel, Carston R. Wagner

- 1:06 Paper 311c: Tandem CAR for Enhancing Antitumor Efficacy and Persistence of CAR T Cells in Solid Tumor Treatment
- **Xianhui Chen**, Jiangyue Liu, Yun Qu, Pin Wang
- **1:24** Paper 311d: The Presence of an Endothelial Lumen Drives Fungal Germination and Neutrophil Migration in a Physiologically Relevant *in Vitro* Model of Infection
- **Laurel Hind**, Nancy Keller, David J. Beebe, Anna Huttenlocher
- **1:42 Paper 311e:** Developing a Novel Parkinson's Disease Diagnostic
- **Benjamin Schlichtmann**, Anumantha Kanthasamy, Vellareddy Anantharam, Surya K. Mallapragada, Manohar John, Balaji Narasimhan
- **2:00 Paper 311f:** Factor Releasing Regenerative Bandages for Enhanced Healing in Diabetic Wounds
- Sahar Rahmani, Georgios Theocharidis, Evan J. Thompson, Selena Zhang, Konstantinos Kouna, Ting-Yu Shih, Aristidis Veves, David J. Mooney

2:18 Paper 311g: Invited: Engineering Protein Assemblies for Precision Health: Artificial Antigen Presentation and Epitope Discovery

- Fei Wen

(312) Applications in Sensors: Wearables and Environmental

Tuesday, Nov 12, 12:30 PM
Hyatt Regency Orlando, Celebration 10
Kevin J. Cash, Chair
Yi Zhang, Co-Chair
Dongmei (Katie) Li, Co-Chair

Sponsored by: Sensors

12:30 Paper **312a**: Invited: Wearable Fabric Sensor for Determination of Sodium Ions in Sweat

— Hanieh Ghadimi, Chelsea Monty

12:55 Paper 312b: Understanding How Pollution Episodes Affect Community-Level Air Quality with a Distributed Sensor Network

— **Kerry Kelly**, Wei Xing, Pascal Goffin, Tofigh Sayahi, Tom Becnel, Pierre-Emmanuel Gaillardon, Anthony Butterfield, Miriah Meyer, Ross Whitaker

1:12 Paper 312c: Novel Chromogenic Sensors Enabled By Multi-Stimuli-Responsive Shape Memory Polymers — Peng Jiang, Calen Leverant

1:29 Paper 312d: Real-Time Monitoring of Supercritical Hydrocarbon Fuels

— Andrew L. Wagner, Andrew Carpenter, William Reily, Paul E. Yelvington

1:46 Paper 312e: Polymer Thin Film Platforms for the Rapid Detection and Analysis of Waterborne Radionuclides — Scott M. Husson, James C. Foster, Abenazar Darge, Timothy A. DeVol, Brian A. Powell

2:03 Paper 312f: Real-Time Membrane Permeability Measurements of Hydrogen Sulfide and Acetone

— **Reza Shekarriz**, Anastasios Angelopoulos, Nancy Kanagy

2:20 Paper 312g: Ultra-Stretchable Conductive Polymer Complex As a Wearable Strain Sensor with Excellent Linearity and Repeatable Autonomous Self-Healing Ability

— Yang Lu, Jesse Horne, Lauren McLoughlin, Rachel Ploeger, Ju-Won Jeon**, Evan K. Wujcik**

2:37 Paper 312h: CVD Polymers for Early Detection of Huanglongbing (HLB) in Citrus

— **Maxwell Robinson**, Karen Gleason

(313) Area Plenary: Area 8A
Emerging Areas in Polymer Science
and Engineering II (Invited Talks)
Tuesday, Nov 12, 12:30 PM
Hyatt Regency Orlando, Celebration 5
Muzhou Wang, Chair

Allie Obermeyer, Co-Chair Sponsored by: Polymers

12:30 Paper 313a: Artificial Protein Networks

— Lawrence J. Dooling, Joshua Baccile, **David A. Tirrell** **1:05** Paper 313b: Coacervation of Sequence Controlled Polypeptides: Understanding Biology and Designing Materials

— **Sarah L. Perry**, Li-Wei Chang, Tyler Lytle, Whitney C. Blocher McTigue, Abigail Cabral, Shari Traiger, Charles E. Sina

1:40 Paper 313c: Designing High-Performance Block Polymer-Based Membrane Adsorbers for Water Purification

- Bryan W. Boudouris

2:15 Paper 313d: Understanding Effects of Polymer Architecture on Structure and Thermodynamics in Polymer Solutions Using Theory and Simulations

— **Arthi Jayaraman**, Thomas Gartner III, Michiel G Wessels

(314) Bioinspired Membranes and Membrane Processes

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Barrel Spring I Zhongyi Jiang, Chair Manish Kumar, Co-Chair Ronald Michalsky, Co-Chair

Sponsored by: Membrane-Based Separations

12:30 Paper 314a: Bioinspired Pervaporation Membranes

— Hao Yang, Hongjian Wang, Meidi Wang, Guanhua Liu, Hong Wu, Fusheng Pan**, Zhongyi Jiang**

12:51 Paper 314b: Membrane Protein Nanosheet Based Membranes

— Yu-Ming Tu, Woochul Song, Tingwei Ren, Yuexiao Shen, Ratul Chowdhury, Prasangi Rajapaksha, Tyler E. Culp, Alina Thokkadam, Drew Carson, Yuxuan Dai, Arwa Mukthar, Miaoci Zhang, Dibakar Bhattacharyya, William A. Phillip, Enrique D. Gomez, Robert J. Hickey, Yinan Wei, Manish Kumar

1:12 Paper 314c: A pH-Responsive TFC NF Membrane with Rechargeable Anti-Bacterial Property and High Efficient Dye/Monovalent Salt Separation Via Catechol/Boronate Complexation

— Thi Dao Nguyen, Yi Ming, Yan Wang

1:33 Paper 314d: Expected
Performance and Potential Design
Strategies for Highly Selective
Biomimetic Desalination Membranes
— Jay R. Werber, Cassandra Porter,
Menachem Elimelech

1:54 Paper 314e: Bioinspired Membrane Pores Containing Phospholipid Bilayer for Immobilized Enzymatic Catalysis

— Anju Kumari**, Saurav Datta**

2:15 Paper 314f: Modelling of Fluid Transfer in Nanoporous Carbons with Molecular Dynamics Simulation

- Shanshan Wang

2:36 Paper 314g: Forming Water-Wire Networks and Achieving Aquaporinlike Water Permeability and Water/ Salt Selectivity Using Artificial Water Channels

— **Woochul Song**, Himanshu Joshi, Ratul Chowdhury, Yuexiao Shen, Jun-li Hou, Aleksei Aksimentiev, Manish Kumar

(315) Bionanotechnology Graduate Student Award Session I

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Discovery 45 Catherine A. Fromen, Chair Elizabeth Nance, Co-Chair Lorraine Leon, Co-Chair

Sponsored by: Bionanotechnology

12:30 Paper 315a: Award Submission: Directed Evolution of the Optoelectronic Properties of Synthetic Nanomaterials

— **Benjamin Lambert**, Alice Gillen, Nils Schuergers, Shang-Jung Wu, Ardemis A. Boahossian

12:50 Paper 315b: Award Submission: Process Intensification for Small Molecule Synthesis Via Recombinant Peptide Templated Palladium and the Elimination of Intermediate Purification — Imann Mosleh, Robert Beitle, M. Hassan Beyzavi

1:10 Paper 315c: Award Submission: Nanoparticle Carrying T Cells for Targeted Drug Delivery

— **Muhammad Raisul Abedin**, Yongjian Liu, Sutapa Barua

1:30 Paper 315d: Award Submission: Systemic Dendrimer-Mediated Delivery of Triptolide Specifically to Tumor-Associated Macrophages Improves Efficacy in Glioblastoma

— **Kevin Liaw**, Rishi Sharma, Sujatha Kannan, Rangaramanujam Kannan

1:50 Paper 315e: Award Submission: Carbon Nanomaterials Enable Plant Genome Engineering without Transgene Integration

— **Gozde Sultan Demirer**, Huan Zhang, Juliana Matos, Abhishek Aditham, Brian Staskawicz, Markita Landry

2:10 Paper 315f: Award Submission: Self-Assembly of Hydrophobically-Patterned Charged Polypeptides for Drug Delivery — Sara Tabandeh, Lorraine Leon

2:30 Paper 315g: Award Submission: Rational Selection of Intestinal Permeation Enhancers for Oral Macromolecular Drug Delivery — Katherine Fein, Kathryn A. Whitehead

(316) Biophysical Properties of Microbes and Microbial Communities Tuesday, Nov 12, 12:30 PM

Tuesday, Nov 12, 12:30 PM
Hyatt Regency Orlando, Celebration 9
Jessica D. Schiffman, Chair
James Wilking, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

12:30 Paper 316a: Invited Speaker: Microbial Biofilms: Structure, Transport, and Dynamics

- James Wilking

12:50 Paper 316b: Invited Speaker: Establishing and Exploiting Biocolloidal Properties of Biofilms

- Elizabeth J. Stewart

1:10 Paper 316c: Inoculum Concentration As an Independent Variable to Evaluate Biofilm Structure-Function Relationships

— Kirsten Parratt, Joy Dunkers, Heidi Leonard, Nancy J. Lin

1:30 Paper 316d: Invited Speaker: Biofilm Rheology

- Travis W. Walker

1:50 Paper 316e: Invited Speaker: Mechanical Principles of Biofilm Formation

— Jing Yan

2:10 Paper **316f:** Invited Speaker: Role of Chemotactic Adaptation in *H. Pylori* Invasion and Colonization

- Pushkar Lele

2:30 Paper 316g: Diatom Microbubbler for Active Biofilm Removal in Confined Spaces

— Yongbeom Seo, Jiayu Leong, Jun Dong Park, Yu-Tong Hong, Sang-Hyon Chu, Cheol Park, Dong Hyun Kim, **Yu-Heng Deng**, Vitaliy Dushnov, Joonghui Soh, Simon Rogers, Yi Yan Yang, Hyunjoon Kong

(317) Characterization of Composites Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 11

Ioannis Zuburtikudis, Chair Yifan Li, Co-Chair Yanbin Xu, Co-Chair

Sponsored by: Composites

Focatiis, Michael J. Bortner

12:30 Paper 317a: Insights into Frictional Properties of Carbon Fiber Epoxy Composites Characterized Using Parallel-Plate Rheometry

— *Arit Das, David A. Dillard, Davide De*

12:55 Paper 317b: Diffusion-Softening of a Mechanically Adaptive Cellulose Nanocrystal Polyurethane Composite

— Cailego Pritchard, Ignah Fallon

— **Cailean Pritchard**, Jacob Fallon, Michael J. Bortner

1:20 Paper 317c: Titanium Oxide Hydrates As Versatile Species in Inorganic-Organic Hybrids for Light and Heat Management Devices

— Alex Balzer, Natalie Stingelin

1:45 Paper 317d: Using 3D Printing Process Parameters to Assess the Robustness of Cement-Based Printing Material

— **Babajide Y. Onanuga**, Hajar Taheri Afarani, Joseph J. Biernacki

2:10 Paper **317e**: A Comprehensive Analysis of Transient Heat Conduction in Composite Solid Slabs Using Tailor-Made Integral Transforms

- Satish J. Parulekar

2:35 Paper 701b: Multifunctional Biomimetic Nanocoatings from Large Scale One-Step Co-Assembly — Anna Marie LaChance, Sonia Chavez, Jingjing Liu, Songshan Zeng, Luyi Sun

(318) Chemical Engineers in Medicine Plenary II (Invited Talks)

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 12/13

Leonard F. Pease III, Chair Swomitra Mohanty, Co-Chair

Sponsored by: Chemical Engineers in Medicine

12:30 Paper 318a: Anti-Amyloid Failures Increase As Aducanumab for Alzheimer's Disease Flops: A Chemical Engineer's Perspective

— Georges Belfort

1:15 Paper 318b: (All) Things Merge into One: Viral/Nonviral Chimeric Gene Carriers and Chemically-Induced Extracellular Blebs (EBs) for Efficient, Safe, and Versatile Therapies

— Young Jik Kwon

2:00 Paper 318c: Modulation of Drug and Microbe Transport across the Intestinal Mucosal Barrier

– Bhavya Singh, Ian Smith, Oljora Rezhdo, Sigal Saphier-Sharabani, Rebecca L. Carrier

(319) Chemical Modifications and **Processing of Biomaterials**

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Discovery 47 Catherine E. Brewer, Chair Michael T. Timko, Co-Chair

Sponsored by: Forest and Plant **Bioproducts Division**

12:30 Paper 319a: Synthesis and Characterization of Water-Soluble Anionic Carboxvlic Acid-Terminated Lignin Dendrimer for Metal Chelating — Zhaohui Tong**, Shanyu Meng**, Yuncong Li, Yongsheng Chen

12:51 Paper 319b: Functionalized Superparamagnetic Lignin Nanosphere for Phosphate Removal

– Zhaohui Tong**, Tiantian Li**, Yuncong Li

1:12 Paper 319c: Using Soybean Hull in Production of Paper-Based Gas Sensor for Food Packaging Applications

- Navid Etebari Alamdari, Burak Aksoy, Zhihua Jiang

1:33 Paper 319d: The Application of Nonlinear Dynamic Optimization on the Three Pseudo-Components Kinetic Modeling of Biomass (Rhus Typhina) Pyrolysis Using the DAEM - **Hui Liu**, Sajjad Ahmad, Shervin

Sammak, Hesham Alhumade

1:54 Paper 319e: Functional and Chemical Properties of Bio-Oil Produced from Biomass Residues – Mudasir a Shah

2:15 Paper 319f: Efficient Method for Synthesis of High-Value 5-Methylfurfural from 6-Deoxy Sugar in Biphasic System - Ban Heng Sr., You-wei Cheng, Xi Li, Li-jun Wang

2:36 Paper 319g: Reductive Fractionation: Date PALM Biomass to High VALUE Chemicals Using Commercial NiAl Alloy Catalyst - Emmanuel Galiwango, Ali H. Marzouqi, Abbas Ahmed Khalil, Mahdi Abu-Omar

(320) Chromatography Techniques for Bioprocessing

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Barrel Spring II **Nick Merchant, Chair** Stefano Menegatti, Co-Chair

Sponsored by: Bio Separations

12:30 Paper 320a: Separation of Monoclonal Antibody Charge Variants with Continuous Chromatography and Mixed-Mode Resins

- Shu-Ying Jing, Shan-Jing Yao, Dong-Qiana Lin

12:50 Paper 320b: Quantifying Host Cell Protein Interactions with Antibodies Using Interaction Chromatography

- Sarah Hedberg, Daryl Williams

1:10 Paper 320c: Bovine Serum Albumin and Myoglobin Separation By Size Exclusion Simulated Moving Bed Technology

- Albertina Rios, Ana M. Ribeiro, Alirio Rodrigues, Alexandre Ferreira

1:30 Paper 320d: Polymeric Adsorbent for Endotoxin Removal from **Biopharmaceutical Solutions**

Sidharth Razdan, Sutapa Barua

1:50 Paper 320e: Flow-through Chromatography of Proteins As a Continuous and Integrated Separation Method

- Chyi-Shin Chen, Noriko Yoshimoto, Shuichi Yamamoto

2:10 Paper 320f: Preparation of a Novel Tetrapeptide Biomimetic Chromatographic Resin and Its High Antibody-Binding Capacity

- Yu-Ming Fang, Dong-Qiang Lin, Shan-Jing Yao

2:30 Paper 320g: Production and Isolation of Phospholipids from Microalgae for Formulation of **Green Cosmetics**

- Ahmet Y. Manisali, Aydin K. Sunol, George Philippidis

(321) Concentrated Solar Energy for Power Generation and Chemical **Processing II**

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Regency Ballroom T Alexandre Yokochi, Chair Nick AuYeung, Co-Chair Wojciech Lipinski, Co-Chair Christopher L. Muhich, Co-Chair

Sponsored by: Concentrated Solar Energy for Power Generation and **Chemical Processing**

12:30 Paper 321a: Gasification of Organic Solid Waste Under High-Flux Solar Irradiation: Thermodynamics, Kinetics, and Fixed-Bed Reactor Evaluation

- Xian Li, Ye Shen, Wojciech Lipinski, Yanjun Dai, Chi-Hwa Wang

12:55 Paper 321b: Analysis of the Effect of Solar Pyrolysis Parameters on the Physicochemical Properties of Biochar

- Alejandro Ayala-Cortés, Diego R. Lobato-Peralta, Carlos E. Arreola-Ramos, Diana C. Martínez-Casillas, Daniella E. Pacheco-Catalán, Ana K. Cuentas-Gallegos, Heidi I. Villafán-Vidales, Camilo A. Arancibia-Bulnes

1:20 Paper 321c: Numerical Design and Experimental Evaluation of a Direct Solar Reactor for the Catalytic Dry Reforming of Methane

- Tayseir Mohammed, Jawad Sarwar, Konstantinos E. Kakosimos

1:45 Paper 321d: Economic and Dynamic Performance Solar-Driven Thermochemical Production of Hydrogen Using Ceria

- Alicia Bayon, Alberto de la Calle

2:10 Paper 321e: Dish-STARS™ Solar Thermochemical Production of Hydrogen

- Richard Zheng, Robert Wegeng, Paul Humble, Johnny Saavedra-Lopez, Timothy Veldman

(322) Continuous Drug Substance Isolation

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 6 Andreas S. Bommarius, Chair David A. Acevedo, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 322a: Continuous Synthesis, Crystallization, and Isolation of Amoxicillin

- Matthew A. McDonald, Ronald W. Rousseau, Martha A. Grover, Andreas S. **Bommarius**

12:51 Paper 322b: Continuous Centrifugal Extraction for Intermediate Recovery from a Biocatalysis Reaction - Joseph Imbrogno, Steven M. Guinness, Rajesh Kumar, Andrew Derrick, Emma McInturff, Mark Guinn

1:12 Paper 322c: Continuous Mixing/ Washing of an API Suspension in a Precipitating Environment - Isabella Aigner, Manuel Zettl, Manuel Kreimer, Thomas Mannschott, Peter van der Wel, Johannes G. Khinast, Markus Krumme

1:33 Break

1:54 Paper 322e: Multistage, Multi-Zones Antisolvent-Cooling Crystallisation of a Proprietary API: Comparison of Two Continuous Crystalliser

- **Ebenezer Ojo**, Humera Siddique, Ali Anwar Ian Houson Ruairi O'Meadhra Berthold Schenkel, Alastair Florence

2:15 Paper 322f: Continuous Crystallization Using Mixed Suspension Mixed Product Removal (MSMPR) Crystallizers and Oscillatory Baffled Crystallizers (OBC)

- Xiaochuan Yang, David A. Acevedo, Jiaxiang Zhang, Sean Naimi, Jiahao Wu, Sonal Mazumder, Celia N. Cruz, Thomas O'Connor

2:36 Paper 322g: Risk Assessment of Encrustation in Continuous Pharmaceutical Crystallization Process a Case Study

- David A. Acevedo, Xiaochuan Yang, Jiaxiang Zhang, Sonal Mazumder, Thomas O'Connor, Rapti Madurawe, Celia N. Cruz

(323) Data-Driven Design and **Modeling of Biomaterials**

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Peacock Spring Yi He, Chair

Reid C. Van Lehn, Co-Chair Qing Shao, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

12:30 Paper 323a: Data-Driven Design of Self-Assembling Pi-Conjugated Oligopeptides (Invited Talk) Kirill Shmilovich, Andrew Ferguson

1:06 Paper 323b: Data-Driven Design of Functional Amyloid Biomaterials - Sai Vamshi R Jonnalagadda, Shujun He, Joseph M. Jakubowski, Asuka A. Orr, Xue L. Lim, Chrysoula Kokotidou, Manos Gkikas, Anna Mitraki, **Phanourios Tamamis**

1:24 Paper 323c: Exploration of Interresidual Contacts in Combined Coarse Graining and Experiment Directed Simulations of AB42 - Dilnoza Amirkulova, Andrew White,

Heta Gandhi

1:42 Paper 323d: Conjugation of DOPA and Amyloid Structures for Molecular Design of Underwater Adhesives

- **Amelia Chen**, Qing Shao, Carol Hall

2:00 Paper 323e: Optimizing Antifreeze Protein Activity Via an Elitist Genetic Algorithm: A Comparison of High and Low Activity Variants - Daniel J. Kozuch, Frank H. Stillinger, Pablo G. Debenedetti

- 2:18 Paper 323f: Development of Polymeric Vehicles for Gene Delivery Using High-Throughput Experimentation and Statistical Learning
- **Ramya Kumar**, Ngoc Le, Zhe Tan, Theresa M. Reineke
- **2:36** Paper 323g: The Effect of Heteromultivalency on Lectin-Glycan Binding Process and the Identification of Critical Parameter
- **Hyun-Kyu Choi**, Dongheon Lee, Singla Akshi, Joseph Sang-Il Kwon, Hung-Jen Wu

(324) Data-Driven Techniques for Dynamic Modeling, Estimation, and Control II

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 25 Daniel Chen, Chair Kirti M. Yenkie, Co-Chair

Sponsored by: Systems and Process Control

- **12:30 Paper 324a:** Adaptive Corrective Strategies Via Integrated Data-Driven Monitoring and Explicit Fault-Tolerant Control
- **Baris Burnak**, Melis Onel, Efstratios N. Pistikopoulos
- **12:48** Paper 324b: Model Identification and Disturbance Forecasting Via Recurrent Neural Networks for Building Applications
- Matthew J. Ellis
- **1:06** Paper **324c:** Data-Driven Input Design to Maximize Information in MIMO System Identification
- Kurt E. Häggblom
- **1:24 Paper 324d:** Gaussian Process-Based Optimal Design of Experiments Under Structural Model Uncertainty
- **Panagiotis Petsagkourakis**, Michail Stamatakis, Federico Galvanin
- **1:42** Paper **324e:** Parameter Estimation of Partial Differential Equations Using Artificial Neural Network
- **Elnaz Jamili**, Vivek Dua
- **2:00 Paper 324f:** Grey-Box Identification for a Class of Nonlinear Dynamical Systems
- **Robert J. Lovelett**, Ioannis G. Kevrekidis
- 2:18 Paper 324g: Space-Time
 Dynamics of Electricity Markets
 Incentivize Technology Decentralization
 Yue Shao, Victor M. Zavala
- 2:36 Paper 324h: Model Predictive Control-Assisted Online Data Collection — *Henrique Oyama*, *Helen Durand*

(325) Design for a Circular Economy Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Regency Ballroom U Shweta Singh, Chair Clayton S Jeffryes, Co-Chair

Sponsored by: Sustainability Science and Engineering

- **12:30** Paper **325a:** Resource-Circular Manufacturing Systems Optimisation *Miao Guo*
- 12:55 Paper 325b: Novel Approach to Material Selection: A Joint Venture of Multiscale Simulations and LCA
- **Andrea Mio**, Domenico Marson, Suzana Aulic, Erik Laurini, Sabrina Pricl, Maurizio Fermeglia
- **1:20 Paper 325c:** Circular Economy Systems Engineering
- **Styliani Avraamidou**, Efstratios N. Pistikopoulos
- 1:45 Paper 325d: A Decision-Making Tool for the Design and Evaluation of Waste Management Systems in Livestock Facilities
- **Edgar Martín-Hernández**, Mariano Martín, Gerardo J. Ruiz-Mercado
- **2:10 Paper 325e:** CAPE: A Circular Economy Perspective
- Edlira Kalemi, Linsey Koo, Nikolaos Trokanas**, Franjo Cecelja**

(326) Education Division Plenary: Award Winners and Perspectives on 10 Years of the Education Division (Invited Talks)

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 22 Matthew Liberatore, Chair Donald P. Visco Jr., Co-Chair

Sponsored by: Education

- **12:30** Paper **326a:** The Myriad Service Opportunities in ChE Teaching and Learning: Find One for You
- Laura P. Ford
- **1:00 Paper 326b:** The Integration of Visualization into Education through Comics and Animation
- Lucas J. Landherr
- 1:30 Paper 326c: "Do I Need to Know This for the Exam?" Shifting Students' Engagement Towards Professional Practice
- Milo D. Koretsky
- **2:00** Paper **326d:** Centering a Community: Building an Aiche Education Division
- David L. Silverstein
- **2:30 Paper 326e:** Education Division: Present and Future
- Matthew Liberatore, Benjamin J. Davis, Daniel Lepek, Taryn Bayles, Katie Cadwell, Priscilla Hill, Shannon Ciston, Daniel D. Burkey

(327) Electrochemical Fundamentals: Faculty Candidate Session

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom J Maureen H. Tang, Chair Xiao Su, Co-Chair

Sponsored by: Electrochemical Fundamentals

- **12:30** Paper **327a:** Toward Solid-State Lithium—Sulfur Batteries through Solid Electrolyte Engineering
- Ankit Agrawal, Brett Helms

- **12:45** Paper **327b**: Electrode-Decoupled Redox Flow Batteries Enable Demand-Conformal Energy Storage
- **Shrihari Sankarasubramanian**, Yunzhu Zhang, Cheng He, Thomas Gregory, Vijay Ramani
- **1:00 Paper 327c:** Understanding the Effects of Polymer Coatings on High Capacity Lithium Metal Anodes
- **Jeffrey Lopez**, Yi Cui, Zhenan Bao
- **1:15 Paper 327d:** Colloidal Nanocrystals As Building Blocks for Electrocatalysis
- Molly Jhong, Delia J. Milliron
- **1:30** Paper **327e:** Ion-Containing Polymers for Suppressing Electrochemical Instabilities in Metal Batteries
- **Snehashis Choudhury**, Yi Cui, Zhenan Bao
- 1:45 Paper 327f: Revolutionizing Energy Storage and Conversion Using Nanostructured Nitrides: Synthesis-Structure-Property Relationships
- Abdoulaye Djire
- 2:00 Paper 327g: A Reduced-Order Physics-Based Calendar Life Model for Li-lon Cells
- **Saeed Khaleghi Rahimian**, M. Mehdi Forouzan, Ying Liu
- 2:15 Paper 327h: Going Beyond Intercalation Capacity of Aqueous Batteries By Exploiting the Conversion Reactions of Mn and Zn-Based Electrodes for Energy Dense Applications
- Gautam G. Yadav
- 2:30 Paper 327i: Mechanistic
 Electrochemistry at the Center of Energy
 Science: From Catalysts to Batteries
 Srini Ramakrishnan, Robert M.
- **Srini Ramakrishnan**, Robert M. Waymouth, Christopher E. D. Chidsey, Bryan D. McCloskey
- 2:45 Paper 327j: Electrochemically Catalyzed Carbon Dioxide Reduction Reactions and Formation Pathways to Two-Carbon and Three-Carbon Molecules on the Metallic Copper Surfaces
- **Zhou Lin**, Kun Jiang, Alejandro J. Garza, Alexis T. Bell, Martin Head-Gordon

(328) Entrepreneurship and Investing in Early Stage Companies Tuesday, Nov 12, 8:00 AM

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom N

Sponsored by: Entrepreneurship in Chemical Engineering - Sponsored by CIEE

- **8:00 Paper 328a:** Investing in University Startups: How to Pick the Winners
- David Mackanic
- **8:30 Paper 328b:** Presentation by Praful Krishna, CEO, Coseer *Praful Krishna*
- **9:00 Paper 328c:** Presentation by Eric Breese, Evonik Venture Capital *Eric Breese*

- **9:30 Paper 328d:** Understanding Venture Capital Funding Decisions and Using Initial Funding to Build a Successful Startup
- Jason Zeng

10:00 Paper 328e: Presentation by Charles Andres, Attorney, WSGR

— Charles Andres

(329) Experiences in Teaching Process Safety I

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 17 Kenneth Cox, Chair Benjamin John Davis, Co-Chair Tracy Carter, Co-Chair

Sponsored by: Product Design

- 12:30 Paper 329a: Risk Assessment in Unit Operations Laboratories

 Tracy Carter, Samira M. Azarin,
 Christopher Barr, M. Jane Brennan, Amy
 J. Karlsson, Sarah Wilson
- **12:55 Paper 329b:** Using Simulators for a Competitive Process Safety Exercise
- **Robert G. Bozic**, Matthew B. Garvey, Donald C. Glaser
- **1:20 Paper 329c:** Classroom Use of Process Simulators to Quantify Flashing Two Phase Release Conditions
- **Thomas O. Spicer III**, Thomas Krumpolc
- **1:45** Paper **329d:** Chemical Engineering Student Moral Reasoning within Hypothetical Process Safety Contexts
- **Jeffrey Stransky**, Daniel Anastasio, Matthew Cooper, Daniel D. Burkey, Cheryl A. Bodnar
- **2:10** Paper 329e: The 4th Edition of Chemical Process Safety, Fundamentals with Applications
- Joseph F. Louvar, Daniel A. Crowl

(330) Flow Assurance and Asset Integrity

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Challenger 40 Vikram Subramani, Chair Kiran Gawas, Co-Chair

Sponsored by: Upstream Engineering and Flow Assurance Forum

12:30 Break

- **12:50 Paper 330b:** Co-Aggregation of Asphaltenes and Inorganic Solids in Diluted Bitumen
- **Weiyi Kong**, Josh Martineau, Yuan Yang, Jingzhou Zhang, Brian Knapper, Samson Ng, Michael P. Hoepfner
- 1:10 Paper 330c: Zero-Resistance Ammetry As a Low Power Approach to Monitor Microbially Influenced Corrosion — Chelsea Monty, Sai Prasanna Chinthala, Joshua Davis, Anwar Sadek,
- **1:30 Paper 330d:** A New Approach for Gas Hydrates Transportability under Multiphase Flow
- Amadeu Sum

John Senko

(331) Fundamental Research in **Transport Processes**

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom I Joel L. Plawsky, Chair

Sponsored by: Transport Processes

- 12:30 Paper 331a: Experiments and Simulations of Microbial Growth in a Rotating Bioreactor
- Joshua A. Adeniran, Mingyang Tan, Shailabh Rauniyar, Rajesh K. Sani, Travis
- 12:48 Paper 331b: Multicomponent Diffusion in Nonionic Micellar Solutions with Very Hydrophobic Solutes
- Nathan P. Alexander, Stephanie R. Dungan, Ronald J. Phillips
- 1:06 Break
- 1:24 Paper 331d: Pool Boiling Heat Transport: A Controlled Process to Form Reduced GO Surfaces from GO with Tunable Surface Chemistry and Morphology
- Aniket Rishi, Anju Gupta, Satish
- 1:42 Paper 331e: Interfacial Instability in Spheres By Resonance
- **Nevin Brosius**, Ranga Narayanan, Kevin Ward, Takehiko Ishikawa, Satoshi Matsumoto, Mike SanSoucie
- 2:00 Paper 331f: On Using the Anisotropy in the Thermal Resistance of Solid-Fluid Interfaces to More Effectively Cool Nano-Electronics
- Xiaoyu Wang, David Venerus, Ishwar K. Puri, Sohail Murad
- 2:18 Paper 331g: Engineering Multicomponent Nanoporous Materials for Spectral Filtering of Heat
- Hannah Kim, Zachary Berquist, Brendon Brown, Andrej Lenert

(332) Fundamentals and Applications for Hazardous Waste Treatment

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Blue Spring I/II Ramesh Chawla, Chair Robert W. Peters, Co-Chair Matthew L. Alexander, Co-Chair

Sponsored by: Solid and Hazardous Waste

- 12:30 Paper 332a: Enhancement of Excess Sludge Hydrolysis with Dielectric Barrier Discharge Plasma Pretreatment – **Qingshuai Meng**, Lecheng Lei,
- 12:42 Paper 332b: Abiotic Degradation with Reactive Iron Mineral Coatings in Anaerobic Sediment
- Lisa Axe, Han Hua, Xin Yin, Wei Ding, Michael Russell
- 12:54 Paper 332c: Nanoparticles for Energy and Environment Applications -Wastewater Treatment
- Ghada Nafie, Gerardo Vitale, Nashaat N. Nassar

- 1:06 Paper 332d: Laboratory Investigation of Combined Chemical/ **Biological Treatment of Hexavalent** Chromium, Carbon Tetrachloride and Trichloroethylene in Aqueous System — Ramesh Chawla, Aadarsh Shah, Md Alamgir Hossain, Michelle Cole, Brady Lee
- 1:18 Paper 332e: Rapid Dechlorination of Polychlorinated Biphenyls (PCBs) in an Engineered System
- Chen Chen, Yang Kun-Lin, Jianzhong He
- 1:30 Paper 332f: Adsorption on NDMA on Biomass-Derived Activated Carbons in Lab-Scale Columns
- Kailev Garland. David Amidei. Catherine E. Brewer, Paul K. Andersen
- 1:42 Paper 332g: Transforming Plastic Waste into Microporous Adsorbents for **Environmental Remediation**
- Xinxin Dong, Baosheng Jin, Cher Hon Lau
- 1:54 Paper 332h: Study of Foam Injection Technology for Soil Remediation Contaminated with Hydrocarbons
- Tomás-Eduardo Chávez-Miyauchi, Mariana Ramirez-Morales
- 2:06 Paper 332i: Facile Ball Milling Method for Developing Surface Functional Groups on Carbon-Based Adsorbents and Their Roles in the Removal of Heavy Metals in Aqueous Solution
- Yulin Zheng, Bin Gao
- 2:18 Paper 332j: Environmentally-Responsible Conversions from Gasification Waste to Energy Storage Devices: Synthesis of Waste-Derived Nanomaterials and Environmental Evaluation
- He Li, Hailin Tian, Xiaonan Wang, Chi-Hwa Wang, Po-Yen Chen
- 2:30 Paper 332k: Ameliorated Phenol Uptake from Paper Mill Effluent Onto Spent Brewer's Saccharomyces Cerevisiae in the Presence of Cetyl Trimethyl Ammonium Bromide
- **Arulmozhi M**, Saravani Natarajan
- 2:42 Paper 332I: Biosurfactant Fermented from Waste Cooking Oil and Its Application on Oil Sludge Celaning
- Chunyan Chen
- 2:54 Paper 332m: Liquid-Liquid Extraction of Chlorophenols from Wastewater Using Hydrophobic Ionic
- Inas M. Alnashef, Reyihangu Sulaiman, Idowu Adeyemi, Shadi Hasan, Shema Abraham

(333) Graphene 2-D Materials: Synthesis, Functions and Applications I

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Discovery 44 Lei Li, Chair Sanjay Behura, Co-Chair

Sponsored by: Carbon Nanomaterials

- 12:30 Paper 333a: High-Yield Scalable **Graphene Nanosheet Production** from Compressed Graphite Using **Electrochemical Exfoliation**
- Thomas Achee, Joshua Hope, Wanmei Sun, Micah J. Green
- 12:50 Paper 333b: Temperature and Gate Dependent Photoresponse in MoS₂-WS₂ Heterostructures
- Rousan Debbarma, Sungjoon Kim, Vikas Berry
- 1:10 Paper 333c: Fabrication of Multi-Dimensional Functional Graphene/ Mxens and Their Industrial Applications - Yidong Liu**, Yong Min**
- 1:30 Paper 333d: How Graphene Nanoribbons Grow during Chemical Vapor Deposition on Ge(001)
- Florian Göltl, Ellen A. Murray, Benjamin Wei Jie Chen, Robert M. Jacobberger, Michael S. Arnold, Manos Mavrikakis
- 1:50 Paper 333e: Increased Electron Transport inside Microbial Fuel Cell through Interfacing Graphene with Geobacter
- Sheldon Cotts, Bijentimala Keisham,
- 2:10 Paper 333f: Reduced Graphene Oxide and Perovskites As Potential Flectrodes for Biomolecular Dve-Sensitized Solar Cells
- Hisham A. Maddah, Vikas Berry, Sanjay Behura
- 2:30 Paper 333g: Wetting Transparency of Graphene on Hydrogel - **Lei Li**, Haitao Liu

(334) Hydrodynamics of Soft and **Active Systems**

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom L Lilian Hsiao, Co-Chair Carlos Silvera Batista, Co-Chair

Sponsored by: Fluid Mechanics

- 12:30 Paper 334a: Hydrodynamics of **Active Chiral Fluids**
- Ming Han, Vincenzo Vitelli, Juan de Pablo
- 12:45 Paper 334b: Upstream Swimming and Taylor Dispersion of Active Brownian Particles
- John Brady, Zhiwei Peng
- 1:00 Paper 334c: Statistical Effects Associated with Tracking Propulsive
- Edmund M. Tang, Patrick T. Underhill
- 1:15 Paper 334d: Bacterial Hopping and Trapping in 3D Porous Media
- Tapomoy Bhattacharjee, Sujit S.
- 1:30 Paper 334e: Rheological Behavior of Soft Particle Glasses during Start-up Flow: Insights from Experiments and Simulations
- Fardin Khabaz, Stefania Traettino, Michel Cloitre, Roger T. Bonnecaze

- 1:45 Paper 334f: Dynamics of Deformable Sheets in Stokes Flow - Yijiang Yu, Michael D. Graham
- 2:00 Paper 334g: The Rheology and Dynamics of Soft Particles in Viscoelastic Flows Via Immersed Boundary **Techniques**
- Christopher Guido, Boon Siona Neo. Eric S. G. Shagfeh
- 2:15 Paper 334h: Revealing the Flow Properties of Polysaccharide-Based Nanostructured Fluids By Microfluidics — Yu-Jiun Lin, Jeffrey S. Horner, Christine Mourafetis, Brandon Illie, Matthew Lynch, Eric M. Furst, Norman J. Wagner
- 2:30 Paper 334i: Nanodroplet Behavior on Soft Substrates
- Fong Yew Leong, Duc-Vinh Le
- 2:45 Paper 334j: Dynamics of Elastic Multi-Compartment Capsules in Microfluidic Channels
- Abdollah Koolivand, Panagiotis **Dimitrakopoulos**

(335) Hydrogel Biomaterials: Cell **Culture and Delivery**

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 16 Steven R. Caliari, Chair Adrianne M. Rosales, Co-Chair Adam Ekenseair, Co-Chair Anita Shukla, Co-Chair

Sponsored by: Biomaterials

- 12:30 Paper 335a: Tunable Three-Dimensional Microarchitecture in Magnetically Templated Hydrogels for Tissue Repair Applications
- Ishita Singh, Zhiyuan Zhao, Christopher Lacko, Mary Kasper, Christine Schmidt, Carlos Rinaldi
- 12:48 Paper 335b: A Comprehensive Study and Comparison of Four Types of Zwitterionic Hydrogels
- Weiqiang Zhao, Lei Zhang
- 1:06 Paper 335c: Antifouling Zwitterionic Hydrogel Coating Improves Hemocompatibility of Activated Carbon Hemoadsorbent
- Qingsi Li, Lei Zhang, Nana Cai
- 1:24 Paper 335d: Bio-Microfluidics Based on Non-Swelling Hydrogels - Chong Shen, Qin Meng
- 1:42 Paper 335e: Development of Injectable Citric Acid-Based Polyester Hydrogel with Sustained Mydgf Delivery Capability for Improved Post-MI Heart Healing
- Xiaoyang Xu
- 2:00 Paper 335f: A 3D Hvaluronic Acid Hydrogel Model for Studying Myelination
- Deniz B. Unal
- 2:18 Paper 335g: A Computational and Experimental Design of Toroidal-Spiral Particles As a Cell Macro-Encapsulation System
- Paola Leon Plata, Colin Foster, Ludwig C Nitsche, Ying Liu

- **2:36** Paper 335h: A Totally Recombinant Fibrin Matrix for Mesenchymal Stem Cell Culture and Delivery
- **Ou Wang**, Ayman Ismail, Frank. M Fabian, Haishuang Lin, Qiang Li, William H. Velander, Srivatsan Kidambi, Yuguo Leo Lei

(336) Industrial Application of Computational and Numerical Approaches to Particle Flow

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 19 Reza Mostofi, Chair Kevin E. Buettner, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

- **12:30 Paper 336a:** Cross-Scale Validation and Evaluation of Wurster Coating Processes
- Thomas Forgber, Stefan Madlmeir, Martina Trogrlic, Adrian Kape, Pankaj Doshi, Alan Carmody, Avik Sarkar, Lourdes Contreras, Johannes G. Khinast, Dalibor Jajcevic
- 12:55 Paper 336b: Simulation and Experimental Validation of a Lagrangian Multiphase Model for Rotary Bell Cup Atomization
- **Wanjiao Liu**, Brandon Petrouskie, Kevin Ellwood, Reza Rock, Seyed Alaie, John Furar
- 1:20 Paper 336c: Multiphase Particle-in-Cell Coupled Population Balance Equation Method for Multiscale Computational Fluid Dynamics
- **ShinHyuk Kim**, Richard D. Braatz, Jay H. Lee
- **1:45** Paper **336d:** Cyclones with and without an Eccentrically Positioned Vortex Finder
- Ray Cocco, Ulrich Muschelknautz, Ben Freireich, S.B. Reddy Karri, T. M. Knowlton
- **2:10 Paper 336e:** Fast CFD Based Optimization of Coal Moving Bed Gasifier
- **Jia Yu**, Liqiang Lu, Mehrdad Shahnam, William A. Rogers
- 2:35 Paper 336f: Large Scale Multiphase Flow Simulation for Techno-Economic Assessment of the Novel Internally Circulating Reactor for Energy Conversion with CO, Capture
- Jan Hendrik Cloete, Mohammed Khan, Schalk Cloete, **Shahriar Amini**

(337) In Honor of Guy Marin's 65th Birthday (Invited Talks)

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Florida Ballroom B Kevin M. Van Geem, Chair Joris W. Thybaut, Co-Chair Mark Saeys, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 337a: Some Industrial Problems Connected to the Research of Guy Marin

— David West

- **12:45** Paper 337b: Chemical Reaction Engineering Future Directions *Jan J. Lerou*
- **1:00** Paper 337c: The Confluence of Kinetic Modeling and Data Science *Linda J. Broadbelt*
- **1:15** Paper 337d: Accurately Predicting Products and Rates of Complex Reacting Systems
- William H. Green
- **1:30 Paper 337e:** Extension of Rigourous Model Fitting for Kinetics into Other Fields
- Hugh Stitt
- **1:45 Paper 337f:** Transient Kinetics in Transition: A Case of Heterogeneous Catalysis
- **Gregory Yablonsky**, Rebecca Fushimi, John T. Gleaves
- **2:00 Paper 337g:** Kinetics-Assisted Design of Supported Noble Metal Catalysts
- Xinggui Zhou
- **2:15 Paper 337h:** Electrochemical Routes to Intensify the Processing of Biomass
- Jonathan Egbert, Michael R. Thorson, **Robert S. Weber**
- **2:30 Paper 337i:** Kinetic-Based Hyperbolic Two-Fluid Models *Rodney O. Fox*
- 2:45 Paper 337j: A Matter of Balancing
- Harry E.A. Van den Akker

(338) Industrial Applications of Computational Chemistry and Molecular Simulation (Invited Talks)

Tuesday, Nov 12, 12:30 PM
Hyatt Regency Orlando, Rock Spring I/II
Phillip R. Westmoreland, Chair
Joseph Golab, Co-Chair
Martin Sanborn, Co-Chair
Jonathan Moore, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

- **12:30 Paper 338a:** Invited Talk By Valeriy Ginzburg
- Valeriy Ginzburg
- **12:55 Paper 338b:** Invited Talk By Agnes Derecskei-Kovacs
- Agnes Derecskei-Kovacs
- **1:20** Paper 338c: Molecular and Detailed Isotopic Structures of Petroleum: Kinetic Monte Carlo Analysis of Alkane Cracking
- **Brian Peterson**, Michael Lawson, Michael J. Formolo
- **1:45 Paper 338d:** Invited Talk By Istvan Lengyel
- Istvan Lengyel
- **2:10 Paper 338e:** Industrial Applications of Materials Informatics
- Richard Ross

- 2:35 Paper 338f: Computing Chemical Reaction Equilibria in Molten Salts from Molecular Simulations: Composition of Molten Carbonate Electrolytes in Contact with Gaseous Species
- Lucas Koziol, Gabor Kiss, Timothy Barckholtz, Jeffrey Young, Anirban Mondal, Athanassios Panagiotopoulos

(339) In Honor of Professor Ignacio Grossmann's 70th Birthday - II (Invited Talks)

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 24 Stratos Pistikopoulos, Chair Nikolaos V. Sahinidis, Co-Chair

Sponsored by: Computers in Operations and Information Processing

- **12:30** Paper **339a**: Ignacio's Legacy in Process Optimization

 Lorenz T. Biegler
- 12:51 Paper 339b: Systems Integration
- **12:51 Paper 339b:** Systems Integration for Advancing Pharmaceutical Manufacturing
- G. V. Rex Reklaitis
- **1:12 Paper 339c:** Title To Be Announced
- Manfred Morari
- **1:33 Paper 339d:** Optimization of the Operation of Integrated, Multi-Plant Systems
- Apostolos Giovanoglou,
 Constantinos C. Pantelides
- **1:54** Paper **339e**: Ignacio Grossmann Turning 70 and Still Going Strong

 Arturo Jiménez-Gutiérrez
- 2:15 Paper 339f: Progress in the Global Optimization of Mixed-Integer Nonlinear Programming Problems — Nick Sahinidis
- **2:36** Comments by former students and other colleagues
- 2:45 Comments by Ignacio Grossmann

(340) Innovations in Particle Engineering: From Amorphous Solid Dispersions to New Processing

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 7 Blair Brettmann, Chair Christopher L. Burcham, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **12:30** Paper 340a: Enhanced Dissolution Performance of Amorphous Solid Dispersions By Size Reduction *Kai Zheng, Rajesh Davé*
- **12:51 Paper 340b:** Modeling Particle Formation in Spray Drying of Amorphous Solid Dispersions
- **Pedro Valente**, Masahiro Nakai, Ricardo Sousa
- **1:12 Paper 340c:** From Liquid to Droplet: Understanding the Ligaments Break-up in Atomization Process
- **Tiago Porfirio**, Francisco J. Galindo-Rosales, Laura Campo-Deano, João Vicente, Viriato Semião

- 1:33 Paper 340d: Analysis of the Microstructure of Particles Obtained By Evaporating Acoustically Levitated Single Droplets Using X-Ray Computed Tomography
- **Hassan Abdullahi**, Christopher L. Burcham, Thomas Vetter
- 1:54 Paper 340e: Decoupling Temperature and the Kinetics of Dye Conversion Via Scalable Nano-Encapsulation in a Thermal-Responsive Media
- **Douglas Scott**, Jie Feng, Madeleine Armstrong, Rodney D. Priestley, Robert K. Prud'homme
- 2:15 Paper 340f: Evaporative Heat Transfer Model for QbD of Agitated Filter Bed Drying
- **Kushal Sinha**, Prashant Kumar, Jie Chen, Raimundo Ho, Laurie Mlinar, Nandkishor Nere
- **2:36** Paper 340g: Novel Co-Processing Technology to Generate Drug Substances Amenable to Direct Compression
- **Deniz Erdemir**, David Buckley, Vivek Daftary, Mark Lindrud, Gregory Lane, Adriene Malsbury, Jing Tao, Nathaniel D. Kopp, Daniel Hsieh, Whitney Nikitczuk, Joshua Engstrom

(341) In Recognition of the 50th Anniversary of ExxonMobil Corporate Strategic Research: SEP (Invited Talks)

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Rainbow Spring I/II Dhaval Bhandari, Chair Ryan Lively, Co-Chair

Sponsored by: Separations Division

- **12:30** Paper 341a: Addressing the Dual Challenge through Advanced Separations: From Materials to Process Scale-up
- Patricia Bielenberg
- **12:55 Paper 341b:** Engineering Low-Energy-Intensive Large-Scale Gas Separations
- William Koros
- **1:20 Paper 341c:** Ionic Liquids for Chemical Separations
- Joan F. Brennecke
- **1:45** Paper **341d:** Sorption Kinetics in MFI- the First Hydrophobic Zeolite *Douglas Ruthven*
- **2:10 Paper 341e:** Process Intensification in Multicomponent Distillation
- **Rakesh Agrawal**, Zheyu Jiang, Radhakrishna Tumbalam Gooty
- **2:35 Paper 341f:** Developing Adsorption Fundamentals for Gas Separation Processes
- **Yu Wang**, Harry W. Deckman, Pavel Kortunov, Peter I. Ravikovitch, Edward Corcoran

(342) Integrated Design for Drug Substance Synthesis

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 8 Joe Hannon, Chair Jason Mustakis, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

12:30 Paper 342a: Kinetic Parameter Estimation from Multiple Spectroscopic Datasets with or without Unwanted Spectral Contributions Using Kipet — Michael Short, Salvador García-Muñoz, Lorenz T. Biegler

12:55 Paper 342b: Using First-Principles and Data-Driven Models to Guide Inference of Pharmaceutical Reaction Data

- Ke Wang, Lu Han, Jason Mustakis

1:20 Paper 342c: Integrating Statistical Analysis and Kinetic Modeling to Increase Learning from High-Throughput Experiments

— **Eric M. Saurer**, Patricia Cho, Victor W. Rosso, Bahar Inankur, Ronald Carrasquillo-Flores, Jacob Albrecht, Frederick Roberts

1:45 Paper 342d: Model Parameter Uncertainty Revisited

- Andrew Bird, Joe Hannon

2:10 Paper 342e: Reaction Kinetic Modeling and Process Optimization of Multi-Enzyme Biocatalytic Cascade Syntheses

— **Kevin Stone**, Jonathan P. McMullen, Shane T. Grosser, Jacob H. Forstater, Gregory Hughes, Ania Fryszkowska, Mark Huffman

2:35 Paper 342g: Understanding of a Continuous Barbier-Type Grignard Process Via Mechanistic Modeling

— **XiaoXiang Zhu**, Elçin İçten-Gençer, Silei Xiong, Jo Anna Robinson, Matthew G. Beaver, Ayman Allian, Amit Goda, Seth Huggins, Pablo A. Rolandi, Shawn Walker, Roger A. Hart

(343) Interfacial and Nonlinear Flows Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom M

Irmgard Bischofberger, Co-Chair Pierre Brun, Co-Chair

Sponsored by: Fluid Mechanics

12:30 Paper 343a: Pattern Formation over Deformable Structures in Confined Geometries

— Christopher Ushay, Etienne Jambon-Puillet, **Pierre Brun**

12:45 Paper 343b: Supramolecular Oscillatory Surface Forces Drive Instabilities in Stratifying Foam Films — Chenxian Xu, Subinuer Yilixiati, Yiran Zhang, **Vivek Sharma**

1:00 Paper 343c: Long-Time Dynamics of Thin Leaky Dielectric Films: Sliding and Cascading Structures

— **Dipin Pillai**, Ranga Narayanan

1:15 Paper 343d: Shock Wave and Hole Formation on a Spreading Liquid Drop — Seungho Kim, Brian Wu, Jason Dombroskie, Sunghwan "Sunny" Jung

1:30 Paper 343e: Breakup Behavior of Droplets with Interfacial Viscosity — Vivek Narsimhan, Natasha Singh, Charlie Lin

1:45 Paper 343f: Vesicle Shape Stability in General Linear Flows

— **Charlie Lin**, Vivek Narsimhan

2:00 Paper 343g: Geometry and Dynamics of Lipid Membranes

— **Amaresh Sahu**, Alec Glisman, Kranthi K. Mandadapu

2:15 Paper 343h: Viscous Fingering in Drying Colloid-Polymer Solutions
— Thitiporn Kaewpetch, Javier Buceta, James F. Gilchrist

2:30 Paper 343i: Active Control of Viscous Fingering Using Electric Field — *Tao Gao*, *Mohammad Mirzadeh*, *Martin Z. Bazant*

2:45 Paper 343j: Pattern Formation from Instabilities in Chromonic Liquid Crystals

— Qing Zhang, Shuang Zhou, **Irmgard Bischofberger**

(344) Machine Learning Applications and Intelligent Systems

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 26 Matthew J. Realff, Chair Chris Kieslich, Co-Chair

Sponsored by: Data and Information Systems

12:30 Paper 344a: Coarse-Scale PDEs from Microscopic Observations Via Machine Learning

— **Seungjoon Lee**, Mahdi Kooshkbaghi, Constantinos I. Siettos, Tom S. Bertalan, Ioannis G. Kevrekidis

12:49 Paper 344b: Machine Learning Methods in Process Control

— Zhe Wu**, Zhihao Zhang**, David Rincon, Panagiotis D. Christofides

1:08 Paper 344c: Application of Deep Neural Networks for Artifact Removal from Sensor Data

— **Mohammad Reza Askari**, Mudassir Rashid, Iman Hajizadeh, Mert Sevil, Sedigeh Samadi, Ali Cinar

1:27 Paper 344d: Nonlinear Dynamic Feature Extraction Based on Gaussian Process Dynamical Models for Jit-Based Adaptive Soft Sensors

— **Yasuhiro Kanno**, Hiromasa Kaneko

1:46 Paper 344e: Attention-Based Recurrent Neural Network for Multi-Step-Ahead Prediction

— **Majid Moradi Aliabadi**, Ming Dong, Yinlun Huang

2:05 Paper 344f: A Deep Reinforcement Learning Approach for Production Scheduling

— Christian D. Hubbs, Nikolaos V. Sahinidis, Ignacio E. Grossmann, John M. Wassick 2:24 Paper 344g: Decision-Making of Online Rescheduling Procedures Using Neuroevolution of Augmenting Topologies

— Teemu Ikonen, Iiro Harjunkoski

2:43 Paper 344h: Progan: Protein Solubility Generative Adversarial Nets for Data Augmentation in Dnn Framework

- Xi Han, Kang Zhou, Xiaonan Wang

(345) Materials and Processes for Thermo-, Electro- and Photo-Chemical Energy Storage - Material Innovations

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Regency Ballroom Q

Anirudh Balram, 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

12:30 Paper 345a: Rare Earth Elements Production from Geothermal Power Plant Using Magnetic Nanofluids — *Jian Liu*, *Michael Sinnwell*, *Paul Martin*, *Praveen K. Thallapally*, *B. Peter McGrail*

12:51 Paper 345b: Adsorption Material for Thermal Energy Storage at Low Relative Humidity Operating Conditions
— *Ye Hua, F. Handan Tezel*

1:12 Paper 345c: Superlocal Equilibrium in Low Temperature Plasma Reactors

— Elijah Thimsen

1:33 Break

1:54 Paper 345e: Effects of Transition Metal Cation Additives on the Passivation of Lithium Metal Anode in Li-S Batteries

— **Wenduo Zeng**, Mark Cheng, Simon Ng

2:15 Paper 345f: Fibrous Conduction Networks Under Various Calendaring Regimes in Electrospun LiFePO₄/C Fibers — Keith Boyle, Venkat R. Bhethanabotla, Sylvia Thomas

2:36 Paper 345g: H₂ Generation Ability of Binary Transition Metal Perovskites via Thermochemical Water-Splitting Process

— Joseph Houck, Vinod S. Amar, **Rajesh Shende**

(346) Micro- and Nano-Scale Technologies in Life Sciences II Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 4 Vamsi K. Yadavalli, Co-Chair Ethan Lippmann, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Paper 346a: Nanomaterials Enable DNA-Free siRNA-Guided Gene Silencing in Intact Plants

— Gozde Sultan Demirer, Huan Zhang, Natalie Goh, Roger Chang, Markita Landry

12:48 Paper 346b: Single-Molecule Conductance Measurements with Conformational Smear Characterization for Nucleotide Recognition

— **Lee Korshoj**, Sepideh Afsari, Anushree Chatterjee, Prashant Nagpal

1:06 Paper 346c: DNA Sample Preparation for Long-Read Genomics Using Microfluidics

— Paridhi Agrawal, Kevin D. Dorfman

1:24 Paper 346d: Breaking Barriers to Practical DNA-Based Information Storage Systems

— Kyle J. Tomek, Kevin Volkel, Kevin Lin, Alexander Simpson, Austin Hass, Zach McCracken, Elaine Indermaur, James Tuck, **Albert Keung**

1:42 Paper 346e: Facile, Scalable Dendritic Cell-Derived Extracellular Blebs for a Cancer Vaccine

— *Melissa Thone*, *Dominique Ingato*,

Anjali Dixit, Young Jik Kwon

2:00 Paper 346f: Differential Effects of Extracellular Vesicles of Lineage-Specific Human Pluripotent Stem Cells on Cellular Behaviours of Isogenic Cortical Spheroids

— **Mark Marzano**, Julie Bejoy, David Meckes, Yan Li

2:18 Paper 346g: A Rapid Method for Label-Free Enrichment of Rare Trophoblast Cells from Cervical Samples — Christina M. Bailey-Hytholt, Sumaiya Sayeed, Morey Kraus, Richard Joseph, Anita Shukla, Anubhav Tripathi

2:36 Paper 346h: Direct Forcing of the Cellular Nucleus Reveals That Transient, Tensile Stresses Can Cause Nuclear Membrane Rupture

— Qiao Zhang, Andrew Tamashunas, Ashutosh Agrawal, Aditya Katiyar, Mehdi Torbati, Richard Dickinson, Jan Lammerding, **Tanmay Lele**

(347) Microbiomes and Metabolomes in Food, Health, and Bioprocessing

Tuesday, Nov 12, 12:30 PM
Hyatt Regency Orlando, Celebration 1
Shang-Tian Yang, Chair
Eirini Velliou, Co-Chair
Xin Xin, Co-Chair

Sponsored by: Food

12:30 Paper **347a**: *Listeria* Biofilm Control Via *Leuconostoc Mesenteroides* Probiotic Isolates

— **Kuili Fang**, Xinhao Shao, Daniel Medina, Jason Wan, Jung-Lim Lee, Seok Hoon Hong

12:48 Paper 347b: Fatty Acids Library Screening and Their Synergistic Effect with Nisin on Inhibiting Biofilm and Persister Formation of *Listeria Monocytogenes*

— **Jiacheng Zhou**, Xing Jin, Kuili Fang, Seok Hoon Hong

- **1:06** Paper 347c: High-Level Antibiotic Tolerance of a Clinically-Isolated Enterococcus Faecalis strain

 Huan Gu, Sweta Roy, Xiaohui

 Theng Dacheng Ren, Huilin Ma, Zafer,
- **Huan Gu**, Sweta Roy, Xiaohui Zheng, Dacheng Ren, Huilin Ma, Zafer Soultan, Christopher Fortner, Shikha Nangia
- **1:24** Paper **347d:** Narrow Spectrum Antibiotic Treatment of *Clostridium Difficile* infection Improves Preservation and Restoration of Intestinal Metabolic Profile
- Karin Yanagi, Kyongbum Lee
- **1:42** Paper 347e: Modeling of Environment-Dependent Microbial Interactions and Dynamics
- **Hyun-Seob Song**, Na-Rae Lee, Kang Zhou, Dong-Yup Lee
- 2:00 Paper 347f: An in silico study of the Metabolic Transactions in the Rumen Microbiome and the Metabolic Shifts Inflicted By Virome Interactions
- **Mohammad Mazharul Islam**, Samodha C. Fernando, Rajib Saha
- 2:18 Paper 347g: Keynote: Combined Effects of Microstructure and Minimal Processing on the Response and Spatial Organization of Listeria in Viscoelastic Models
- Katherine Costello, Hani El Kadri, Jorge Gutierrez-Merino, Madeleine J. Bussemaker, Cindy Smet, Jan Van Impe, Eirini Velliou

(348) Mixing and Segregation of Particulates

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 21 Aaron Morris, Chair Yi Fan, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- **12:30 Paper 348a:** Liquid Transfer between Particles in the Impregnation of Catalysts in a Rotating Drum: Axial Dispersion Studies and the Effect of Particle-Particle Contact
- **Yangyang Shen**, M. Silvina Tomassone, William G. Borghard
- **12:48** Paper **348b:** Effect of Non-Sphericity of Particles on Segregation of Bidisperse Granular Mixture in Lab-Scale Industrially Relevant Systems Using DEM and Experiments
- **Anshu Anand**, Sanjay Verma, Jeetram Yogi
- **1:06 Paper 348c:** Simulation of Flow-Driven Segregation in Mixtures of Disks and Rods
- **Ryan P. Jones**, Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow
- **1:24** Paper 348d: Predicting Granular Density Segregation—a Kinetic Theory Approach
- Yifei Duan, Paul B. Umbanhowar, Julio M. Ottino, **Richard M. Lueptow**

- **1:42 Paper 348e:** Modeling Segregation of Polydisperse Granular Materials in Hopper Discharge Flow
- **Zhekai Deng**, Yi Fan, Jörg Theuerkauf, Karl Jacob, Paul B. Umbanhowar, Julio M. Ottino, Richard M. Lueptow
- 2:00 Paper 348f: Particle Motion in a Vertical Bladed Mixer Using X-Ray Particle Tracking Velocimetry (XPTV) — Humair Nadeem, Shankar Subramaniam, Kushal Sinha, Theodore

J Heindel

- 2:18 Paper 348g: Exploration of the Unique Shear Behavior of Binary Blend Pongpumin Bunchatheeravate, Jiecheng Yang, Jennifer S. Curtis, Joseph W. Bullard
- 2:36 Paper 348h: Segregation Effects in Three Types of Mass Flow Hoppers

 Kerry Johanson

(349) Modeling and Control of Crystallization II

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Coral Spring I/II Zoltan Nagy, Chair Michael Lovette, Co-Chair

Sponsored by: Crystallization and Evaporation

- 12:30 Welcoming Remarks
- **12:33 Paper 349a:** Rapid Screening of Solvents for Crystallization Using Group Contribution Method
- **Anish V. Dighe**, Urmila M. Diwekar, Meenesh R. Singh
- **12:54** Paper **349b**: Dynamic Modelling, Simulation and Optimisation of Batch Enzymatic Amoxicillin Production
- **Samir Diab**, Andrew B. Cuthbertson, Alistair D. Rodman, Dimitrios I. Gerogiorgis
- **1:15** Paper 349c: Dynamic Simulation and Optimisation of Ampicillin Crystallisation
- **Samir Diab**, Antonios Dafnomilis, Andreas G. Boudouvis, Dimitrios I. Gerogiorgis
- **1:36 Paper 349d:** Kinetic Monte Carlo Simulation of Anisotropy in CsPbBr₃ Nanocrystals
- **Niranjan Sitapure**, Tian Qiao, Dongheon Lee, Hyun-Kyu Choi, Joseph Sang-Il Kwon, Dong Hee Son
- **1:57 Paper 349e:** Population Balance Modeling of Cooling-Antisolvent Crystallization to Derisk Tech-Transfer
- Tamar Rosenbaum, **Li Tan**, Niall Mitchell, Michael Dummeldinger, Joshua Enastrom
- 2:18 Paper 349f: A Mathematical Model of the Ultrasound-Assisted Crystallization of Aspirin in a Continuous Tubular Reactor
- **Symeon Savvopoulos**, Mohammed N. Hussain, Jeroen Jordens, Steffen Waldherr, Tom Van Gerven, Simon Kuhn

- 2:39 Paper 349g: Crystal Morphology and Process Control of Multiple High-Salinity Wastewater Via Membrane Distillation Crystallization
- Xiaobin Jiang, Gaohong He, Xuehua Ruan

(350) Molecular Simulation of Adsorption I

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Manatee Spring II

Alexander Neimark, Chair Daniel W. Siderius, Co-Chair

Sponsored by: Adsorption and Ion Exchange

- **12:30** Paper **350a**: Applicability of Generic Force Fields for Adsorbent Screening
- Seulchan Lee, Yongchul G. Chung
- **12:50** Paper 350b: Bottom-up Approach to the Coarse-Grained Surface Model: Effective Solid-Fluid Potentials for Adsorption on Heterogeneous Surfaces *Kaihang Shi, Erik E. Santiso, Keith E. Gubbins*
- **1:10** Paper 350c: Adsorption-Induced Deformation of Faujasite Zeolites: Molecular Simulation Study
- Alina Emelianova, Gennady Gor
- **1:30 Paper 350d:** Impact of Flexiblity on Gas Diffusion in Interpenetrated Metal Organic Frameworks
- **Ravichandar Babarao**, Mahdi Moshref Javadi
- **1:50** Paper 350e: Molecular Models with Accurate Descriptions in Electrostatic Potential for Molecular Simulations of Adsorption
- **Eun Hyun Cho**, Li-Chiang Lin
- **2:10** Paper 350f: 2D Phase Transitions of Fluid Adsorbed in Cylindrical Mesopores: Influence of Adsorbent-Adsorbate Interactions
- **Daniel W. Siderius**, William P. Krekelberg, Vincent Shen
- 2:30 Paper 350g: The Importance of Pore Connectivity in Gas Adsorption Atomistic Simulations for Porous Polymers
- **Dylan Anstine**, Coray M. Colina, Maciej Haranczyk

(351) Multi-Scale Modeling Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom F Andrew J Adamczyk, Chair

Anthony G. Dixon, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 351a: Model-Driven Design of Experiments and Optimization — *Yifan Wang, Ziwei Cheng, Dionisios G. Vlachos*

- **12:50 Paper 351b:** Accelerating Reactive CFD Simulations with Detailed Pyrolysis Chemistry Using Artificial Neural Networks
- **Pieter P. Plehiers**, Laurien A. Vandewalle, Guy B. Marin, Christian V. Stevens, Kevin M. Van Geem
- 1:10 Paper 351c: Building a Microkinetic Model from First Principles for Higher Amine Synthesis on Pd and Co Catalysts
- **Gisela Lozano-Blanco**, Andrew J Adamczyk
- 1:30 Paper 351d: Multi-Scale Modeling of a ZoneFlowTM Structured Catalytic Reactor for Steam Methane Reforming

 Florent Minette, Juis Calamote de
- **Florent Minette**, Luis Calamote de Almeida, Juray De Wilde
- **1:50 Paper 351e:** Generalized Temporal Acceleration Scheme for Kinetic Monte Carlo Simulations of Surface Catalytic Processes
- **Craig Plaisance**, Eric Dybeck, Mie Andersen, Matthew Neurock, Karsten Reuter
- 2:10 Paper 351f: Multi-Scale Reduced Order Models for Real-Time Simulations of Monolith Reactors with Coupled Homogeneous-Catalytic Reactions

 Ram R. Ratnakar, Vemuri
- 2:30 Paper 351g: From Atom to Industrial Reactor: A Multi-Scale Simulation of Syngas Methanation
 Minhua Zhang, He Dong, Kuiwei

Ralakotaiah

— **Minhua Zhang**, He Dong, Kuiwe Yang, Zhongfeng Geng, Yingzhe Yu, Xiuqin Dong

(352) Nanomaterials for Energy Storage I: Li-ion and Li Metal Batteries

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Discovery 46 Ling Fei, Chair Jay Hoon Park, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

- **12:30 Paper 352a:** Metal-Free Carbon Electrocatalysts for Efficient Energy Conversion and Storage

 —Liming Dai
- **1:00** Paper 352b: Nanoparticle Applications for Catalysis

 Chinmay Joshi, Saptarshi Chakraborty
- **1:15** Paper 352c: Investigation of Gel Polymer Electrolyte Failure Mechanism in Lithium-Sulfur Batteries
- **Somayeh Zamani**, George Shebert, Yong Lak Joo
- 1:30 Paper 352d: Mechanisms of Stable Cycling 3D Structured Anodes for High Energy Density Lithium Metal Ratteries
- **Rui Zhang**, Xin Shen, Xiao-Ru Chen, Xiang Chen, Xin-Bing Cheng, Qiang Zhang
- **1:45** Paper 352e: Design and Engineering of Interfaces/Interphases for Stable Li Anodes

 Donghai Wang

- 2:00 Paper 352f: Mechanistic Elucidation and Electrochemical Performance of Amorphous Carbon Interfaced Graphite-Silicon Advanced Apodos
- **Mihit H. Parekh**, Anton Sediako, Ali Naseri, Murray Thomson, Vilas G. Pol
- 2:15 Paper 352g: Silicon Carbide As a Protective Layer to Stabilize Si-Based Anode By Inhibiting the Chemical Reaction
- **Chunhui Yu**, Fei Wei, Chenxi Zhang, Xiao Chen
- 2:30 Paper 352h: Free-Standing Bimetallic Sulfide@Carbon Nanofiber Networks As Lithium-Ion Battery Anodes — Zizhou He, Jed LaCoste, Ling Fei
- 2:45 Paper 352i: Highly Stable Lithium Metal Batteries Enabled By Regulating the Solvation of Lithium Ions in Nonaqueous Electrolytes
- Xue-Qiang Zhang, Xiang Chen, Xin-Bing Cheng, Bo-Quan Li, Xin Shen, Jia-Qi Huang, Qiang Zhang

(353) Oxygen and Hydrogen Photocatalysis and Electrocatalysis II

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Florida Ballroom A Astrid M. Müller, Chair

Mohammad Asadi, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 353a:** Laser-Made Nanocatalysts for Photoelectrochemical Water Oxidation
- Astrid M. Müller
- **12:48** Paper **353b:** A Highly Efficient Fe-Rich Confined Catalyst within Layered Zirconium Phosphate for the Oxygen Evolution Reaction in Alkaline Media
- **Joel Sanchez**, Michaela Burke-Stevens, Meng Zhao, Alex Young, Michal Bajdich, Laurie A King, Thomas F. Jaramillo
- **1:06** Paper 353c: Iridate Perovskites As Highly Active Electrocatalysts for Water Oxidation in Acidic Conditions
- Linsey Seitz
- **1:24 Paper 353d:** Catalyst Development for Oxygen Reduction Reaction
- Samira Siahrostami
- 1:42 Paper 353e: Activity of CoS₂ for Electrochemical Oxygen Reduction Reaction Under Different Reaction Conditions
- **Pallavi Bothra**, Zhiyi Lu, Ambarish Kulkarni, Michal Bajdich, Yi Cui, Jens K. Norskov
- 2:00 Paper 353f: Design of Mixed Metal Oxides for Efficient Intermediate Temperature Oxygen Electrocatalysis — Juliana S. A. Carneiro, Laura Paz Herrera, Xiang-Kui Gu, Eranda Nikolla

- **2:18** Paper 353g: Trends in Oxygen Electrocatalysis of 3d Layered (Oxy) (Hydro)Oxides
- **Zhenghang Zhao**, Philomena Schlexer, Ambarish Kulkarni, Michal Bajdich
- 2:36 Paper 353h: Heterostructure-Promoted Oxygen Electrocatalysis Enables Re-Chargeable Zinc-Air Battery with Neutral Aqueous Electrolyte — *Zhiyong Zhang*, *Li An*, *Sen Zhang*,
- (354) Pharma 4.0 (Invited Talks) Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 27 Nima Yazdanpanah, Chair Christopher L. Burcham, Co-Chair

Sponsored by: Next-Gen Manufacturing

Pinxian Xi

- **12:30 Paper 354a:** Approaches to Knowledge Management and Data Transformations in Pharmaceutical Process Invention
- Jean Tom, Jose E. Tabora
- **1:00 Paper 354b:** Leading the Way to Pharma 4.0
- **Lucas Vann**, Amos Dor, Amy Doucette
- **1:30** Paper 354c: Machine Learning in Pharmaceutical Process Development: Where Are We up to in Pharma 4.0?
- John Mack
- **2:00 Paper 354d:** Digital Twins, Microfactories and People for Future Pharmaceutical Manufacturing
- Cameron Brown
- **2:30 Paper 354e:** The Art of the Possible When Digitising Your Pharmaceutical Operations
- Scott Lawson

(355) Polymers for Energy Storage and Conversion

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Celebration 15 Ian Hosein, Chair Jian Qin, Co-Chair

Sponsored by: Polymers

- **12:30 Paper 355a:** Electrodeposition of Metals in Cross-Linked Polymer Electrolytes
- Lynden A. Archer
- **1:00 Paper 355b:** Understanding Interfacial Effects on Ion-Transport in Block Copolymer Electrolytes
- **Michael Webb**, Juan de Pablo
- 1:12 Paper 355c: Biohybrid Photoelectrode Made from Photosynthetic Protein Complex Psi Entrapped within a Semi-Conducting Tcnq-Based Charge-Transfer Film
- **Tyler Bennett**, Dibyendu Mukherjee, Bamin Khomami
- **1:24 Paper 355d:** Enhancement of the Interfacial Bonding Strength of Nafion for a Novel PEM Fuel Cell Architecture
- **Pei-Kang Sun**, R. S. Besser

- **1:36** Paper **355e:** Impact of Solvation Energy on the Morphological Behavior of Ion-Containing Copolymers
- Kevin Hou, Jian Qin
- 1:48 Paper 355f: Predicting the
 Performance of Lithium Metal Electrodes
 Stabilized By Polymer Electrolytes
- **Nitash P. Balsara**, Jacqueline Maslyn
- **2:00** Paper 355g: Decoupling Mechanical Properties and Ion Conductivity in Supramolecular Stretchable Battery Materials
- **David Mackanic**, Xuzhou Yan, Yi Cui. Zhenan Bao
- **2:12 Paper 355h:** Aramid Nanofiber Separators for Energy Storage
- Anish Patel, Kathryn Wilcox, Ian George, Rishabh Juneja, Zhuo Li, Christina Lollar, Simone Lazar, Jaime C. Grunlan, Hongcai Zhou, Wyatt Tenhaeff, Jodie L. Lutkenhaus
- 2:24 Paper 355i: Influence of Dopants on the Electrochemical Properties of Conducting Polymers As Electrodes for Supercapacitors
- **Miaomiao Zhang**, Amit Nautiyal, Haishun Du, Xinyu Zhang
- **2:36** Paper **355**j: Coarse-Grained Model of Energy Transport in Disordered Conjugated Polymer Network
- Elizabeth M. Y. Lee, Juan de Pablo
- 2:48 Paper 355k: Solid Polymer Ionics: Nanostructure Design for Solid-like Mechanics and Liquid-like Ion Transport — Snehashis Choudhury, Lynden A.

(356) Population Balance Modeling for Particle Formation Processes: Nucleation, Aggregation and Breakage Kernels

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 20 Dana Barrasso, Chair R. Bertrum Diemer Jr., Co-Chair

Sponsored by: Particle Production and Characterization

- 12:30 Paper 356a: Analysis of Nanoparticle Growth and Aggregation in Non-Thermal Plasma and Plasma Afterglow By Advanced Ion Mobility Spectrometry and Monte Carlo Simulation
- **Xiaoshuang Chen**, Takafumi Seto, Uwe R. Kortshagen, Christopher J. Hogan Jr.
- **12:55** Paper **356b**: Model Identification Using in-Line Estimates of Crystal Size *Roberto Irizarry, Jochen Schoell, Lorenzo Codan*
- 1:20 Paper 356c: Population Balance Modeling for Twinscrew Granulation: Insight in the Notion of Distance between Distributions and the Need for Identifiable Models for Good Predictive Power
- **Daan Van Hauwermeiren**, Thomas De Beer, Ingmar Nopens

- **1:45** Paper **356d**: Detailed Population Balance Modelling Using a Hybrid Particle Model
- **Astrid Boje**, Jethro Akroyd, Markus Kraft
- **2:10** Paper 356e: Spherical Agglomeration Process: Mechanistic Understanding and Mathematical Modelling
- Omid Arjmandi-Tash, Jonathan D. Tew, Siti N. Mohd Yusoff, Kate Pitt, James D. Litster, **Rachel M. Smith**
- **2:35 Paper 356f:** Mechanism Discrimination Based on Population Balance Models
- R. Bertrum Diemer Jr.

(357) Process Intensification and Modular Manufacturing: Fundamentals and Applications

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 28 Fereshteh Farzad, Chair Ignasi Palou-Rivera, Co-Chair

Sponsored by: Process Intensification & Modular Chemical Processing

- **12:30** Paper 357a: Intensification of Ammonia Production

 Mahdi Malmali
- **12:55 Paper 357b:** Sensitivity of Desulfurization Cost for Small-Scale Natural Gas Sweetening Units
- Yushi Deng, Shuang Xu, Selen Cremaschi, Mario Richard Eden, Kylie Webb, Harrison Wright, Paul S. Dimick
- **1:20 Paper 357c:** Dynamic Intensification of Ternary Distillation Columns
- **Lingqing Yan**, Thomas F. Edgar, Michael Baldea
- **1:45** Paper **357d:** Integrated Mechanical Vapor Compression-Membrane Distillation for Treating High Salinity Produced Water: Progress and Update
- Mahdi Malmali
- **2:10** Paper 357e: Towards Safe and Operable Process Intensification Systems *losif S. Pappas*, *Yuhe Tian, Justin Katz, Baris Burnak, Styliani Avraamidou, Efstratios N. Pistikopoulos*

(358) Refining and Petrochemical Plant Modelling and Operations Improvements

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Challenger 38/39

Vladimir Mahalec, Chair Mark L. Darby, Co-Chair Wenli Du, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

- **12:30 Paper 358a:** Optimization of C₃MR LNG Liquefaction Process Using a Parallelized Simulator
- **Trevor Rice**, Yoshitsugi Kikkawa, Mingder Lu
- **12:51** Paper **358b**: Study on Advanced Control for Natural Gas Dehydration Plant *Md Emdadul Haque*, *Qiang Xu*, *Srinivas Palanki*

- 1:12 Paper 358c: Novel Piecewise Linearization of Rigorous Nonlinear Natural Gas Transportation Model for Optimal Network Operation
- Kody Kazda, Xiang Li
- **1:33 Paper 358d:** Simulation of Pressure Swing Adsorbers Using the Moving Bed Model
- **Michael Sees**, Toni Kirkes, Taehun Kim, Joseph Scott, Chau-Chyun Chen
- **1:54** Paper 358e: Correlation between the Yield of Deasphalted Oil and Hansen Solubility Parameter of Its Feedstock in a Solvent Deasphalting Process
- Junwoo Park, Ki Bong Lee
- 2:15 Paper 358f: New Digital Method Enables Flexibility, Production, and Reliability Improvements While Mitigating Overhead Corrosion from Tramp Amines
- -Collin Cross
- 2:36 Paper 358g: Study on Wave Motion Effects on FLNG Mixed Refrigeration Process Via Integrated CFD and Process Simulations
- Xingchun Wang, Qiang Xu

(359) Structured Adsorbents: Beyond Pellets and Beads

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Manatee Spring I Armin D. Ebner, Chair Joeri Denayer, Co-Chair

Sponsored by: Adsorption and Ion Exchange

- **12:30 Paper 359a:** Exploiting Structured Bed Thermal Conductivity for Enhancing the Performance of Temperature Swing Adsorption Processes
- **Pravin B.C.A. Amalraj**, Armin D. Ebner, James A. Ritter
- **12:50** Paper **359b**: On the Use of Structured Adsorbents in Ptsa Cycles for CO₂ Removal from Spacecraft Cabins *Armin D. Ebner, Pravin B.C.A. Amalraj, Ryan T Sanders, James A.*
- **1:10** Paper 359c: Amine-Functionalized MIL-101 Monoliths for CO₂ Removal from Enclosed Environments
- **Shane Lawson**, Connor Griffin, Kambria Rapp, Ali Rownaghi, Fateme Rezgei
- **1:30 Paper 359d:** 3D-Printed ZIF-8 Structured Adsorbents for Biobutanol Recovery
- **Benjamin Claessens**, Jasper Lefevere, Steven Mullens, Gino Baron, Julien Cousin-Saint-Remi, Joeri Denayer
- **1:50** Paper **359e**: Significance of Flow Mal-Distribution and Channel Imperfections in Structured Monolith-Based Adsorption Processes
- Ishan Sharma, Roberto Mennitto, Daniel Friedrich, **Stefano Brandani**

- **2:10** Paper 359f: Development of a 3D-Printed Honeycomb Monolith Adsorbent for CO₂ Capture with Electric Swing Adsorption Process
- Maria João Regufe, Alexandre Ferreira, José Miguel Loureiro, Alírio E. Rodrigues, Ana M. Ribeiro

(360) Technology Transfer and Industrial-Academic Interfaces Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom E Brandon O'Neill, Chair Sarika Goel, Co-Chair

Joshua A. Schaidle, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 360a:** Zeolite Catalysts and Adsorbents in the Oil Industry: Turning Oil into Energy
- **Ivy D. Johnson**, Tilman Beutel, Nadya Hrycenko, Barbara Carstensen
- **12:50** Paper **360b**: Commercialization of Ionic Liquid Acid Alkylation Technology
- **Matthew Cole**, Elizabeth Carter, Hye Kyung Timken
- 1:10 Paper 360c: A Mechanistic Investigation into Basic Metal Oxide Co-Catalyst Functionality in Methanol Conversion Reactions
- Doron Levin
- **1:30 Paper 360d:** Industrializing Atomic Layer Deposition for Upgraded Catalysts: Scale-up Perspectives
- **David M. King**, Arrelaine A. Dameron, James E. Trevey, Jeffrey W. Elam, Christopher L. Marshall
- **1:50** Paper 360e: Triptane Production in a Pilot Reactor: Opportunities and Challenges in Scaling High Octane Gasoline Technology Beyond the Bench
- **Jesse E. Hensley**, Stephane Marie-Rose, Daniel A. Ruddy, Earl Christensen, Jon Luecke, Connor Nash, Joshua A. Schaidle
- **2:10** Paper **360f**: Scale up Strategies for a Novel Biomass Pyrolysis Process *A. R. (Tony) Cartolano*
- 2:30 Paper 360g: Practical Methods for Screening Catalyst for Reforming Applications
- Joshua E. Middaugh

(361) The Food-Energy-Water Nexus Tuesday, Nov 12, 12:30 PM

Hyatt Regency Orlando, Regency Ballroom V Vikas Khanna, Chair Yuan Yao, Co-Chair M. M. Faruque Hasan, Co-Chair

Sponsored by: Sustainability Science and Engineering

12:30 Paper 361a: Spatial Optimization for Land Use Allocation Under Food-Energy-Water Nexus Conciderations

— **Yaling Nie**, Styliani Avraamidou, Xin Xiao, Efstratios N. Pistikopoulos, Jie Li

- **12:55 Paper 361b:** Managing Technological and Ecological Systems in a Watershed While Considering the FEW Nexus, Ecological Carrying Capacity, and the Effects of Climate Change
- **Kyuha Lee**, Sami Khanal, Bhavik R. Bakshi
- **1:20 Paper 361c:** Abfews: An Ammonia-Based System for Food-Energy-Water Sustainability
- Matthew J. Palys, Anatoliy Kuznetsov, Andrew Allman, Joel Tallaksen, Michael Reese, Prodromos Daoutidis
- 1:45 Paper 361d: Comparing the Environmental Implications of National Food Supplies Using Data Envelopment Analysis
- Elysia Lucas, Gonzalo Guillén-Gosálbez, Miao Guo, Carlos Pozo Fernández, Ángel Galán Martín
- **2:10** Paper 361e: Systematic Design and Optimization of Water-Energy Nexus for Sustainable Regional Planning
- **Spyridon D. Tsolas**, M. Nazmul Karim, M. M. Faruque Hasan
- **2:35** Paper 361f: A Computational Platform for Assessing Organic Waste Management Strategies in the Food-Energy-Water Nexus
- **Yicheng Hu**, Gerardo J. Ruiz-Mercado, Rebecca Larson, Victor M. Zavala

(362) Thermal Energy Storage Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 29/30 Masahiro Kawaji, Chair Ryan Anderson, Co-Chair

Sponsored by: Transport and Energy Processes

- **12:30** Paper 362a: Incorporation of a Phase Change Material into Fibers for Thermal Modulation and Energy Storage *Yun-Ho Ahn, Ryan Lively*
- 12:55 Paper 362b: Latent Heat Trapping in Phase Switching Liquids — Rukmava Chatterjee, Daniel Beysens, Sushant Anand
- **1:20** Paper 362c: High Pressure High Temperature Thermal Energy Storage Systemfor Concentrated Solar Power (CSP) Plants
- Masahiro Kawaji
- 1:45 Paper 362d: Flame-Retardancy and Thermal Properties of a Novel Phosphorus Modified PCM for Thermal Energy Storage
- Renjie Chen, DeLong Xie, Dedong He, Xinzhi Chen, Yuanzhi Zhu, Yanping He, Yi Mei
- **2:10 Paper 362e:** Novel Materials for Cold Energy Storage
- **Ali A. Alnajjar**, Husam A. Al-Araj, Daniel Bahamon, TieJun Zhang, Lourdes F. Vega, Maryam Khaleel

- 2:35 Paper 362f: Experimental Study on Thermal Performance of a Latent Heat Thermal Storage Cell Unit Utilizing Finned Metal Foam
- **Yongping Huang**, Ying Yang, Liangyu Wu, Chengbin Zhang

(363) Thermochemical CO₂ Reduction I: C1 Products

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom D Qinghe Zheng, Chair Meenesh R. Singh, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 363a:** Understanding the Activity and Selectivity of Methanol Production from CO₂
- **Pallavi Bothra**, ¹Julia Schumann, Verena Streibel, Frank Abild-Pedersen, Jens K. Norskov
- **12:48 Paper 363b:** Dual Function Material for the Capture and Catalytic Conversion of CO₂ to Fuel from an O₂-Containing Flue Gas
- **Chae Woon Jeong**, Martha A. Arellano, Robert Farrauto
- **1:06 Paper 363c:** Methanol Synthesis from CO₂ Hydrogenation with Ru/Mo Bimetallic Phosphides
- **Feiyang Geng**, Yolanda Bonita, Matthew Magiera, Jason C. Hicks
- **1:24** Paper 363d: The Activation of CO₂ By UiO-66 MOFs in CO₂ Hydrogenation — *Haoxi Jiang, Qiang Gao, Shutian* Wang, Yifei Chen, Minhua Zhang
- **1:42** Paper 363e: Computational Exploration of CO₂ Hydrogenation to Methanol Catalyzed By a Frustrated Lewis Pair within a Defective Uio-66 *Kuiwei Yang*, *Jianwen Jiang*
- 2:00 Paper 363f: Reverse
 Microemulsion Synthesized
 Molybdenum and Cobalt Carbides for
 Thermocatalytic Conversion of CO₂ to
 Renewable Natural Gas and Syngas
 Yue Yu, Guanjie Sun, David Simakov
- 2:18 Paper 363g: Thermal Management of CO₂ methanation Process Based on Experimental and Numerical Approach Using Ni-YSZ Tubular Catalysts
- Fumihiko Kosaka, Toshiaki Yamaguchi, Yuji Ando, Takehisa Mochizuki, Hideyuki Takagi, Koichi Matsuoka, Yoshinobu Fujishiro, Koji Kuramoto
- 2:36 Paper 363h: On the Role of Reverse Water Gas Shift Reaction in Catalytic CO₂ Hydrogenation over Ruand Ni-Based Catalysts
- **Gabriella Garbarino**, Paola Riani, Maria Flytzani-Stephanopoulos, Guido Busca

(364) Thermophysical Properties and Phase Behavior

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Silver Spring

Erik E. Santiso, Chair Clare McCabe, Co-Chair Sanket A. Deshmukh, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 364a: Area 1a Plenary — *Monica Olvera de la Cruz*

1:12 Paper 364b: Developing SAFT-gamma Mie Models for Aqueous Electrolytes: Organic Salts and CO₂-Brine Mixtures

— **Spiros Kournopoulos**, Srikanth Ravipati, Georgia Lazarou, Silvia Di Lecce, George Jackson, Amparo Galindo

1:30 Paper 364c: A Universal Equation of State for Hard Polyhedra

— **Thi Vo**, Sharon C. Glotzer

1:48 Paper 364d: Systematic Evaluation of Thermophysical Properties of Low GWP Refrigerants and Blends for Refrigeration Cooling Systems By Molecular Modeling Techniques

— Carlos Albà-Garriga, Wael A. Fouad, Fèlix Llovell, **Lourdes F. Vega**

2:06 Paper 364e: Systematic Development of an Artifact-Free SAFT Eos

— J. Richard Elliott Jr.

2:24 Paper 364f: Liquid-Liquid Equilibria for Ternary Systems Limonene + Linalool + Ionic Liquid with Lactate Anion — Hiroyuki Matsuda, Yoshihiro Inoue,

— **Hiroyuki Matsuda**, Yoshihiro Inoue, Rina Sakuta, Daisuke Sato, Kiyofumi Kurihara, Katsumi Tochigi

2:42 Paper 364g: Equation of State of the One-Dimensional Lennard-Jones System: Thermodynamics and Fluctuations

— **J. Matthew Mansell**, Erik E. Santiso, Keith E Gubbins

(365) Tribute to Jacob Israelachvili I (Invited Talks)

Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom K Norma Alcantar, Chair Younjin Min, Co-Chair Kai Kristiansen. Co-Chair

Sponsored by: Interfacial Phenomena

12:30 Paper 365a: Direct
Measurement of Forces between
Poly(sodium-4-styrene sulfonate)
Brushes on Mica Immersed in
Aqueous Solutions of Poly(vinyl benzyl
trimethylammonium nitrate)

— **Matthew V. Tirrell**, Dean Mastropietro

1:00 Paper 365b: The Role of Intermolecular and Surface Forces on the Kinetics and Thermodynamics of Bacterial Adhesion

— Shuhao Liu, Michael Bae, Yagmur Yegin, Shifeng Huang, Jun Kyun Oh, Younjin Min, **Mustafa Akbulut** 1:20 Paper 365c: Developing Multifunctional Soft Materials through Tunable Intermolecular and Surface Interactions

- Hongbo Zeng

1:40 Paper 365d: Interaction Forces between Random Coil Proteins

— **Xavier Banquy**, Buddha Ratna Shrestha, Benoit Liberelle, Frederic Murschel, Gregory Decrescenzo

2:05 Paper 365e: Effect of Roughness on Interactions between Surfaces

— **Mark Robbins**, Joseph Monti, Lars Pastewka

2:35 Paper 365f: Measurements of the Mechanical Properties of Paper
— Patricia McGuiggan, Andrea Hall, Thomas OConnor

(366) Understanding Mixing Processes I: Advances in CFD and Computational Analysis Tools Tuesday, Nov 12, 12:30 PM Hyatt Regency Orlando, Bayhill 32 Jason J. Giacomelli, Chair

Sponsored by: North American Mixing Forum

12:30 Paper 366a: Use of the Hierarchical Parcel Swapping Method to Simulate Turbulent Subgrid Reacting Flows with Variable Schmidt Numbers — *David O. Lignell, Victoria B.*

Stephens, Isaac Wheeler

12:51 Paper 366b: Computational Fluid Dynamics Simulations of Mixing in the Transition Region

— **David G. Foster**, Zachary J. Oliver, Paul W. Steve, Riley D. Flower, William T. Funkenbusch

1:12 Paper 366c: Using GPUs to Run Large Eddy Simulations of Blending in Oil Storage Tanks

— **Brian DeVincentis**, John A. Thomas, Kevin Smith

1:33 Paper 366d: The Effect of Grid Cell Type in Mixing Time Simulations in Non-Turbulent Stirred Vessels

- Harry E.A. Van den Akker

1:54 Paper 366e: Analyzing Reactive Mixing Processes Using Computational Fluid Dynamics and *Z*-Transform

— De-Wei Yin

2:15 Paper 366f: Modeling Polymer Fluid Flow and Reaction with Computational Fluid Dynamics (CFD) — Lu Zhu, Jie Jiang, Li Xi

2:36 Paper 366g: CFD-Based Multi-Objective Optimization of Dual-Impeller Configurations in a Gas-Liquid Stirred Tank

— Miao-Na Chen, **Jia-Jun Wang**, Xue-Ping Gu, Lian-Fang Feng

(367) Ammonia Combustion Tuesday, Nov 12, 1:45 PM Hyatt Regency Orlando, Regency

Sponsored by: Ammonia Energy

Ballroom P

1:45 Paper 367a: Duiker Combustion Engineers BV - Stoichiometry-Controlled Oxidation (SCO) Technology for Industrial Ammonia Combustion

- Albert Lanser

2:08 Paper 367b: Pure Ammonia
Combustion Micro Gas Turbine System
— Osamu Kurata, Norihiko Iki, Takahiro
Inoue, Tadahiro Fujitani, Yong Fan,
Takayuki Matsunuma, Taku Tsujimura,
Hirohide Furutani, Masato Kawano,
Keisuke Arai, Ekenechukwu Chijioke
Okafor, Akihiro Hayakawa, Hideaki
Kobayashi

2:31 Paper 367c: Ignition Delay Times of Diluted Mixtures of Ammonia/ Methane at Elevated Pressures — C. Filipe Ramos, Bo Shu, Ravi

Fernandes, Mário Costa

2:54 Paper 367d: Performance of Ammonia/Natural Gas Co-Fired Gas

Turbine with Two-Stage Combustor
— Masahiro Uchida, Shintaro Ito,
Toshiyuki Suda, Toshiro Fujimori

3:17 Paper 367e: New Technology of the Ammonia Co-Firing with Pulverized Coal to Reduce the NOx Emission

— **Takamasa Ito**, Hiroki Ishii, Juwei Zhang, Sakiko Ishihara, Toshiyuki Suda

(368) The Current State of STEM Inclusion in the Workplace

Tuesday, Nov 12, 2:00 PM Hyatt Regency Orlando, Bayhill 23 Anthony Butterfield, Co-Chair Stephanie Farrell, Co-Chair Gayle Gibson, Co-Chair

Sponsored by: Engineering for Inclusion

(369) Interactive Session: Applied Mathematics and Numerical Analysis Tuesday, Nov 12, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

Yash Puranik, Chair Joseph Scott, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

Paper 369a: SMBLtoODEpy: A Software Program for Converting SBML Models into ODE Models in Python

— **Steve M. Ruggiero**, Ashlee N. Ford Versypt

Paper 369b: Towards Field Wide Production Optimization for Upstream Field Recovery: A Holistic Analysis and Optimisation Framework of the Upstream Field from Reservoir to Host Facility

- Shakeel Ramjanee

Paper 369c: GPU-Accelerated Flow Simulations in Mesoporous Source Rocks with Many-Body Dissipative Particle Dynamics

— **Yidong Xia**, Ansel Blumers, Zhen Li, Lixiang Luo, Yu-Hang Tang, Joshua Kane, Hai Huang, Matthew Andrew, Milind Deo, Jan Goral Paper 369e: Optimal Bayesian Experiment Design for Constrained Nonlinear Dynamic Systems Using Stochastic Surrogate Models — Joel Paulson, Marc Martin-Casas, Ali Mesbah

Paper 369f: Numerical Simulation to Predict Motor Bearing Damage By Electrical Pulses

— **Yu Miao**, Alexandre Yokochi, Annette von Jouanne, Ryan Collin, Madeline Stephens, Brian Thayil

Paper 369g: Model-Based Hazard Monitoring and Process Safety Control Using Model Predictive Control — *Qingqing Xu*

Paper 369h: Determine Mixing Effects
Onto the Polymeric Microstructure of
Ldpe with a Compartmentalized HybridNumerical-Stochastical Model
— Oliver Salman, Markus Busch

Paper 369i: Multiple Experts: Using the Mahalanobis Metric to Fuse Data from Different Partial Observations

— **David Sroczynski**, Felix Dietrich, Mahdi Kooshkbaghi, Ioannis G. Keyrekidis

Paper 369j: Dissipative Particle Dynamics Model for Flow Past a Circular Obstacle in a Microchannel at Low Reynolds Number

— **Waqas Waheed**, Anas Alazzam, Ashraf N. Al-Khateeb, Eiyad Abu Nada

Paper 369k: Modeling and Simulation of a Fixed Bed Reactor for CO₂ Capture through Methanation Using Open-Source Software

— **Santiago Ortiz Laverde**, Manuel A. Figueredo Medina, Camilo Rengifo Gutiérrez

Paper 369I: Finding All Solutions of Systems of Nonlinear Equations with an Efficient Global Homotopy Continuation Method

— **Saeed Khaleghi Rahimian**, J. D. Seader

Paper 369m: Comparison of Finite
Volume and Lattice Boltzmann Methods
for Simulations of Multicomponent Flows
— Orest Shardt

Paper 369n: A Control Strategy for Thermostating and Barostating Molecular Dynamics Simulations — Shih-Han Wang, Luke E. K. Achenie

(370) Interactive Session: Data and Information Systems

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S Fani Boukouvala, Chair

Sponsored by: Data and Information Systems

Paper 370a: Computer Vision Improvised Cell Detection for Lab-on-a-Chip Diagnostics Point Care Solutions — Sagar Srinivas, Vishnu Masampally, Venkataramana Runkana Paper 370b: Probabilistic PCA for Multivariate Process Monitoring and Comparison with PCA

- Weike Sun, Richard D. Braatz

Paper 370c: A Holistic Approach for the Development and Test of an Information System

- Holger Mayer, Georg Fieg

Paper 370d: A Data-Driven Approach for Parameter Estimation of Stochastic Models By Using Machine Learning Techniques

— **Chunbing Huang**, Federica Cattani, Federico Galvanin

Paper 370e: Hybrid Cutpoint Optimization Using Improved Swing-Cut Method and Data Analytics for Crude-Oil Distillation Towers

— **Robert E. Franzoi**, Brenno C. Menezes, Jeffrey D. Kelly, Jorge A. W. Gut, Ignacio E. Grossmann

Paper 370f: Quantitative Evaluation of Grouping Complex Substances and Sorbent Material Design: Delivering Data-Informed Insights

— **Burcu Beykal**, Melis Onel, Lan Zhou, Fred A. Wright, Timothy D. Phillips, Ivan Rusyn, Efstratios N. Pistikopoulos

Paper 370g: Experimental Validation of Methods for Optimizing Remaining Useful Life (RUL)

— Jose O. A. Matias, Adriaen Verheyleweghen, Johannes Jäschke

Paper 370h: Prediction of Pressure Drop of Platforming Exchanger in a Continuous Catalytic Reforming Unit — Fangyuan Ma, Tianshu Chen, Jingde Wang, Wei Sun

Paper 370i: Constrained Parameter Identification Algorithms for Dual-Rate Systems with Inter-Sample Output Prediction

— Jingwei Gan**, Satish J. Parulekar**

Paper 370j: A Stochastic Programming for Optimal Fence Line Monitoring and Detection of Toxic and Flammable Gases Using Fixed and Mobile Sensors

Dongil Peter Shin, Dongho Kwak

Paper 370k: Hierarchical Multi-Class Segmentation for Identification of MIMO Systems from Historical Data

— **S. Manikandan**, Raghunathan Renaaswamv

Paper 370I: Semi-Automatic Method to Optimize Multi-Lamp High Flux Solar Simulators Utilizing Machine Learning Algorithms

— Ali Arshard, Safeer Hafeez, Mohammed Hassan, Bassam Khalil, Mohammed Al-Hashimi, Konstantinos E. Kakosimos

Paper 370m: Machine Learning for Biorefining: Towards a Universal Kinetic Model of Wood Deconstruction

— **Yankai Cao**, Heather L. McKenzie-Trajano, Edward Wang

Paper 370n: Constructing Interpretable and Accurate Model Combining Decision Tree and Random Forest

- Naoto Shimizu, Hiromasa Kaneko

Paper 370o: New Evaluation Method of Soft Sensors Considering Characteristics of Time Series Data

— **Takumi Kojima**, Hiromasa Kaneko

Paper 370p: Model-Based Optimization of Laser-Reduced Graphene with Sparse Datasets

— Alexander Tyrrell, Hud Wahab, Vivek Jain, Lars Kotthoff, **Patrick A. Johnson**

Paper 370q: Reverse Mapping of Nonlinear Process Responses By a Trained Neural Network

— Tapan Bagchi

Paper 370r: Development of an Image Analysis Tool for High-Speed Imaging Data in a Dropwise Additive Manufacturing Process

— **Andrew J. Radcliffe**, Gintaras V. Reklaitis

Paper 370s: GPU Parallel Forward and Backward Selection for Model Building

— **Benjamin Sauk**, Nikolaos V. Sahinidis

Paper 370t: Going through the Disruptive Transformations in Chemical Industrial Practices: Impact of Expert Systems and Artificial Intelligence on Automation and Decision Making

— Chandra Shekar Besta Sr., Shivashish Kulshreshtha**, Raju Yerolla**

Paper 370u: Cognitive Autonomous Agents for Process Abnormal Behaviour Detection: An Application of Artificial Intelligence

— **Vishnu Masampally**, Sagar Srinivas, Venkataramana Runkana

Paper 370v: Machine Learning-Based Surrogate Modeling and Optimization: Application to Systematic Process Intensification Using Building Block Superstructure

— **Sun Hye Kim**, Salih E. Demirel, Jianping Li, M. M. Faruque Hasan, Matthew Realff, Fani Boukouvala

(371) Interactive Session: Systems and Process Control

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Victor M. Zavala, Chair Cara Touretzky, Co-Chair

Sponsored by: Systems and Process

Paper 371a: Integrated Mathematical Models for Freshwater Bodies and Constructed Wetlands as Tools for Restoration Planning Through an Optimal Control Approach

— Amira Siniscalchi, Jimena A. Di Maggio, Vanina Estrada, **Maria Soledad Diaz**

Paper 371b: Optimal Control of a Fluid Bed Dryer Granulator Using Near Infrared Sensing with Advanced Process Control

Julián J. Navas González, Carlos
 Velazquez

Paper 371c: Particle Size Control Using Model Predictive Control for a Spray Drying Process

— Christian Barreto-Hernandez, Carlos Velazquez

Paper 371d: Process Monitoring Based on Mutual Information—Multiblock Rolling Pin Vine Copula

— Qiong Jia, Yang Zhou, Shaojun Li

Paper 371e: Nonlinear and Non-Gaussian Process Monitoring Based on Vine Copula and Robust Auto-Encoder Model

- Yang Zhou, Qiong Jia, Shaojun Li

Paper 371f: Conceptual Framework for Integrated Control and Design of Coupled Processes

— Andreas Himmel, Kai Sundmacher

Paper 371g: Stabilization-Oriented Learning Algorithm for Optimal Control of Nonlinear Control-Affine System

— Yeonsoo Kim, Jong Min Lee

Paper 371h: Nonlinear Model Predictive Control of a DC-DC Boost Converter with Constant Power Load: Classical and Explicit Approaches

— **Oswaldo Andrés-Martínez**, Jonathan Mayo-Maldonado, Antonio Flores-Tlacuahuac

Paper 371i: An Efficient Approach to Solving Stochastic Optimal Control Problems with Application to Sustainability Assessment of a Complex Integrated Model

— Pablo T Rodriguez-Gonzalez, **Vicente Rico-Ramirez**, Urmila M. Diwekar

Paper 371j: Handling Bounded and Unbounded Unsafe Sets in Control Lyapunov-Barrier Function-Based Model Predictive Control of Nonlinear Processes

— **Zhe Wu**, Panagiotis D. Christofides

Paper 371k: Multi-Rate Data-Driven
Models for Lactic Acid Fermentation Parameter Identification and Prediction
— Jinawei Gan. Satish J. Parulekar

Paper 371l: The Evolution of Approximated Kinetic Model Structures — *Marco Quaglio*, *Eric S. Fraga*, *Federico Galvanin*

Paper 371m: The Development of Multiparametric Model Predictive Controllers Via the Argonaut Framework

— **Justin Katz**, Burcu Beykal, losif S. Pappas, Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos

Paper 371n: Estimator Based Inferential Control for C₄ Splitting Process Using t-Sne Algorithm and Artificial Neural Network

— **Seungsik Cho**, Minsu Kim, Hyungjoon Yoon, Junghwan Kim, II Moon

Paper 371o: Observer-Based Adaptive Fuzzy Controller for Uncertain Nonstrict Nonlinear Systems with Unknown Control Directions Subject to Input and State Time Delays,Input Saturation

— Antonios Armaou, Mahdi Khajeh Talkhoncheh Paper 371p: Time-Varying Model Identification of Nonlinear Systems with Partially Known Model Structure: Application to NFkB Signaling Pathway Induced by LPS and BFA

— **Dongheon Lee**, Arul Jayaraman, Joseph Sang-Il Kwon

Paper 371q: Modeling and Advanced Process Control of Supercritical Carbon Dioxide (sCO₂)-Based Energy System — Gaurav Mirlekar, Jacob Albright, Shuyun Li, Eric A. Liese, Stephen E. Zitney, Anthony P. Burgard

Paper 371r: Dynamic Optimization of a Natural Gas Combined Cycle (NGCC) Power Plant for Load-Following Operation

— **Yifan Wang**, Debangsu Bhattacharyya, Richard Turton

Paper 371s: Optimizing Tight Oil Recovery through a Single Well Alternating Production-Injection Procedure

— Guofan Luo, Christine Ehlig-Economides, **Michael Nikolaou**

Paper 371t: Structural Evolution of the Electricity System in a below 2°C World — *Habiba A. Daggash*, *Niall Mac Dowell*

Paper 371u: Optimal Heating Profiles in Tubular Reactors with Solid-Phase Axial Wall Conduction for Isothermal Operation

— **Sunjeev Venkateswaran**, Benjamin Wilhite, Costas Kravaris

Paper 371v: Technology Value and Techno-Economic Criteria of Unicorn Technology for Carbon Capture and Sequestration for Electricity System Decarbonisation

— Yoga Wienda Pratama, Niall Mac Dowell

Paper 371w: Dynamic Modeling and Simulation of the Material Stress Profile in a Supercritical Pulverized Coal Boiler Under Load-Following Operation

— **Katherine Reynolds**, Elijah Hedrick, Parikshit Sarda, Benjamin P. Omell, Stephen E. Zitney, Debangsu Bhattacharyya

Paper 371x: Enterprise Wide Optimization of an Integrated Oil and Gas Company: Detailed Transportation and Simplified Refinery Models Integration

- Luis Hoyos Sr.

Paper 371y: Gray-Box Model for Predicting Crystal Radius and Crystal Growth Rate of 300 mm Czochralski Single-Crystal Silicon Ingot Production Process

— **Shota Kato**, Sanghong Kim, Manabu Kano, Toshiyuki Fujiwara, Masahiko Mizuta, Shinji Hasebe

Paper 371z: Design and MULTI-Objective Optimization of an Esterification Reaction and Separation to Production of Riodiesel

— Camilo Monroy-Peña, Anderson Imbachi, Carlos A M Riascos, Paulo César Narváez Rincón, Gustavo Buitrago Hurtado Paper 371aa: Disruptive Artificial Intelligence (Reinforcement Learning) Based Predictive Control

— **Sagar Srinivas**, Vishnu Masampally, Venkataramana Runkana

Paper 371ab: Polyolefin Process Modeling and Monitoring

— Niket Sharma, Y. A. Liu

Paper 371ad: Adaptive Model Predictive Control with Scenario-Based Reference Optimization for Artificial Pancreas Systems

— **Iman Hajizadeh**, Tor Aksel N. Heirung, Ali Mesbah, Ali Cinar

Paper 371ae: Uncertainty and Disturbance Estimator (UDE) Based Model Predictive Control for Optimal Operation of Desulfurization Process — Shan Liu, Wenqi Zhong, Li Sun, Xi Chen

Paper 371af: Simultaneous Model Structure Identification, Parameter Estimation and Process Optimization Via Output Modifier Adaptation

— **Jose O. A. Matias**, Johannes Jäschke

Paper 371ag: Economic Model-Based Controller Design Framework to Optimize Shale Gas Production and Water Management in Hydraulic Fracturing

— **Kaiyu Cao**, Prashanth Siddhamshetty, Yuchan Ahn, Rajib Mukherjee, Joseph Sang-II Kwon

Paper 371ah: A Control Methodology for CO₂ Injection to Optimize Tight Oil Production from a Fractured Horizontal Well

— Guofan Luo, Christine Ehlig-Economides, **Michael Nikolaou**

Paper 371ai: Water Content Detection in Wood Chips By Near Infrared Reflectance

- Forest Dewberry, Kerul Suthar

Paper 371aj: Simulation Software for the Assessment of Nonlinear and Adaptive Multivariable Control Algorithms

— **Mudassir Rashid**, Sediqeh Samadi, Mert Sevil, Mohammad Reza Askari, Iman Hajizadeh, Ali Cinar

Paper 371ak: Enhancing Total Fracture Surface Area in Naturally Fractured Unconventional Reservoirs Via Model Predictive Control

— **Prashanth Siddhamshetty**, Parth Bhandakkar, Joseph Sang-II Kwon

Paper 371al: Model Predictive Control in Continuous Biomanufacturing Utilizing In-Line Process Analytical Tools

— **Sobhana Sripada**, Rajan Bhawnani, Sushmitha Krishnan, Aparajith Bhaskar, Eduardo Lopez-Montero, John Mack, Jessica R. Molek

(372) Interactive Session: Systems and Process Design

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

M. M. Faruque Hasan, Chair Charles C. Solvason, Co-Chair

Sponsored by: Systems and Process Design

Paper 372b: Model-Based Identification of Process Operational Design Space Under Uncertainty

— Panagiotis Demis, **Oleksiy V. Klymenko**

Paper 372c: Process Design Automation Using Reinforcement Learning
— Damdae Park, Jaehyun Shim, Jong

Paper 372d: A Simulation-Based Superstructure Optimization Approach for Process Synthesis and Design Under Uncertainty

— **Resul AI**, Krist V. Gernaey, Gürkan Sin

Paper 372e: Involving the Water-Energy-Waste Nexus in the Optimal Design of Total Integrated Residential Complexes

— **Jesús M. Nuñez-López Sr.**, Eusiel Rubio-Castro, José María Ponce-Ortega

Paper 372f: Cost-Driven Heat Exchanger Network Synthesis Covering Practical Implementation Issues

– Matthias Rathjens, Georg Fieg

Paper 372g: A Nonsmooth Formulation for Representing Unclassified Process Streams in Work and Heat Exchange Networks (WHENs)

— **Matias Vikse**, Harry A. J. Watson, Paul I. Barton, Truls Gundersen

Paper 372h: Optimal Synthesis of Cooling Water Systems

— **Ricardo F.F. Pontes**, Giovanna M.L.M. Franco, Evelin K.G. Silva

Paper 372i: Involving Economic Incentives in Optimizing the Methanol Supply Chain Considering Conventional and Unconventional Resources

— Esbeydi Villicaña, José M. Ponce, Mahmoud El-Halwagi

Paper 372j: Life Cycle Analysis of the Syngas-to-Aromatics Processes

— Wenlong Song, Yilin Hou, Dali Cai, Zhaohui Chen, Weizhong Qian

Paper 372k: Air Pollutant Emissions and Regulatory Implications of Co-Processing Raw Bio-Oil in U.S. Petroleum Refineries

— Arpit Bhatt, Yimin Zhang

Paper 3721: The Influence of Renewable Penetration on Optimal Planning and Scheduling of Industrial Utility Plants: Economics, Environmental Impact, Flexibility and Resiliency

— Chuan Zhang

Paper 372m: Development of Deep Direct-Use Geothermal System on West Virginia University Campus-Morgantown, WV

— **Nagasree Garapati**, Oluwasogo Alonge Paper 372n: Contribution of Upcycling Surplus Hydrogen to Design of a Sustainable Supply Chain: The Case Study of Northern Spain

— Yanez Maria, **Alfredo Ortiz**, Braulio Brunaud, Ignacio E. Grossmann, Inmaculada Ortiz

Paper 372o: Optimal Energy Storage in Batteries: A Convex Formulation for Definition of Charge/Discharge Schedules

- Mariana Corengia, Ana I. Torres

Paper 372p: Optimal Design and Operation of Biomass Waste Gasification for Energy and Biochar Production — Xin He, Zhiyi Yao, Chi-Hwa Wang

Paper 372q: The Use of Process Graph for the Design of Pyrolysis

Oil Biorefinery Superstructure, and Optimization in Terms of Cost — *Anamaria Paiva Pinheiro Pires*, *Manuel Garcia-Perez*

Paper 372r: Systematic Framework for Solvent Recovery, Reuse, and Recycling in Industries

— **John Chea**, Amanda Christon, Vanessa Pierce, Maxim Russ, Jake Stengel, Stewart Slater, Mariano Savelski, Kirti M. Yenkie

Paper 372s: Alternative Generation and Evaluation Using a Design Framework: Case Study on Drug Substance Manufacturing Processes of Biopharmaceuticals

— **Haruku Shirahata**, Sara Badr, Hirokazu Sugiyama

Paper 372t: Simultaneous Optimization of Rigorous Reactor Design and Process Synthesis: Application to Direct CO₂ Conversion of Methanol

— **Hee Won Lee**, Jonggeol Na, Honggon Kim, Ung Lee

Paper 372u: Simulated Moving Bed Chemical-Looping Combustion Reactor for Power Generation in Combined Cycle Power Plants

— Chen Chen, George M. Bollas

Paper 372v: General Techno-Economic Analysis for Electrochemical Coproduction of CO₂ Reduction and Anodic Oxidation

— Jonggeol Na, Bora Seo, Jeongnam Kim, Hyung-Suk Oh, **Ung Lee**

Paper 372w: Microkinetic Model Reduction for Ethylene Oligomerization Reactor Optimization and Design

— Kanishka Ghosh, Alexander W. Dowling

Paper 372x: Spacing Design for Active Sorting of Drops in Millifluidic Network: A Genetic Algorithm-Based Approach

— **E.M. Arun Sankar**, Faiz K. Mohammed, Mohammad Shahab, Raghunathan Rengaswamy

Paper 372y: Integration of Molecular Simulations and Computer-Aided Molecular Design to Enable Novel Azeotropic Separations

— **Bridgette Befort**, Alexander W. Dowling, Edward Maginn

Paper 372z: A Shortcut Model for Multicomponent Azeotropic Distillation Column Design

— Zheyu Jiang

(373) Interactive Session: Systems and Process Operations

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Sponsored by: Computers in Operations and Information Processing

Paper 373a: On the Design and Solution of an Online Scheduling Optimization for Open-Loop and Closed-Loop Strategies

— **Robert E. Franzoi**, Brenno C. Menezes, Jeffrey D. Kelly, Jorge A. W. Gut

Paper 373b: Analysis of Carbon and Water Policies in the Optimal Design of Water Distribution Networks Involving Power-Desalination Plants

— Aurora del Carmen Munguía-López, Ramón González-Bravo, José María Ponce-Ortega

Paper 373c: Sequential Dynamic Optimization of Multi-Stage Vacuum Swing Adsorption

— **Zhimian Hao**, Yannic Vaupel, Adrian Caspari, Alexei A. Lapkin, Adel Mhamdi, Alexander Mitsos

Paper 373d: Data-Driven Prescriptive Maintenance Scheduling and Process Optimization

— Christopher Kwadwo Gordon, Melis Onel, Baris Burnak, Efstratios N. Pistikopoulos

Paper 373e: A Computation
Methodology for Energy Storage System
Capacity Under Uncertainty
— Jun-Hyung Ryu

Paper 373f: Scheduling of Baseload Power Plants and Batteries with Integration of Renewables

— Rebecca Kim, Sai Pushpitha Vudata, Yifan Wang, Debangsu Bhattacharyya, Fernando V. Lima, Richard Turton

Paper 373g: GPU Acceleration As Low Cost Enabling Technology for Optimization Based Synthesis of Novel Integrated Crystallizer-Wet Mill Systems — Botond Szilagyi, Zoltan K. Nagy

Paper 373h: Optimization of Water-Energy-Food Nexus Under Uncertainty: A Case Study of Mexico

— **Javier Tovar-Facio**, Victor M. Zavala, Ramón González-Bravo, José María Ponce-Ortega

Paper 373i: A Stochastic Approximation Method for Chance-Constrained Nonlinear Programs

- **Rohit Kannan**, James Luedtke

Paper 373j: Two-Stage Nonlinear Robust Optimization of Effluent Treatment Network Under Uncertainty — Sanjula Kammammettu. Zukui Li Paper 373k: Analysis of the Transient and Limit Distributions of Stochastic Linear Systems with Zonotopic Support

— Mario Eduardo Villanueva, Boris Houska

Paper 373I: A Back-Off Approach for Simultaneous Design and Control for Large-Scale Applications Using an Adaptive Search Space

— Mina Rafiei, Luis A. Ricardez-

Sandoval

Paper 373m: A Multi-Stakeholder Optimization for Total Energy Integrated Systems

– Natali Zarza-Martínez, Luis Fernando Lira-Barragán, José María Ponce-Ortega, Medardo Serna-González

Paper 373n: Application of Multi-**Objective Optimization Using Commercial Process Simulators**

— Fabian Zapf, Thomas Wallek

Paper 373o: Distributionally Robust Optimization Production and Maintenance Schedules

— Johannes Jäschke**, Adriaen** Verheyleweghen

Paper 373p: Effective Systematic Optimization Approach for Integrated Energy Systems: LNG Case Study - Mary Katebah, Mohamad Hussein, Abdulla Al-Hajri, Easa Al-Musleh

Paper 373q: Optimization of Symmetric Problems in Continuous Domain

- **Jianping Li**, M. M. Faruque Hasan

Paper 373r: Optimal Design and Operation of Flexible Energy Polygeneration Systems Using **Decomposition Algorithms** — Avinash Shankar Rammohan

Subramanian, Thomas A. Adams II, Truls Gundersen, Paul I. Barton

Paper 373s: Enhancing Petroleum Field Profitability Via Optimisation of **Production and Injection Operations** — **Emmanuel I. Epelle**, Dimitrios I. Gerogiorgis

Paper 373t: Exploring Energy Landscapes Using the Directed Graph

— Juan Bello-Rivas, Noah J. Wichrowski, Yorgos M. Psarellis, Ioannis G. Kevrekidis

Paper 373u: Approximate Solution to Multi-Parametric Programming Problem Using Robust Optimization

— Said Rahal**, Zukui Li**

Paper 373v: A Mixed Integer Non-Linear **Programming Model for Optimizing** the Operation of a Complex Gas-Oil Separation Network

- Abdullah Al Ghazal, Yufeng He

Paper 373w: Surrogate-Based Optimisation of Integrative Process Systems for Resource Recovery from Wastewater

— Alex Durkin, Marcos Millan, Miao Guo

Paper 373x: Global Optimization of a Class of Black-Box Problems

— Ishan Bajaj, M. M. Faruque Hasan

Paper 373y: Data-Driven Method for Real Time Optimization of Mode-Based Processes

— Gustavo Campos, Ahmet Palazoglu, Yaman Arkun

Paper 373z: Two-Stage Reinforcement Learning for Batch Bioprocess Optimization Under Uncertainty

- Panagiotis Petsagkourakis, E. Antonio del Rio Chanona, Dongda Zhang, Eric Bradford

Paper 373aa: Comparison of Global, Stochastic Optimization Algorithms Using Toy Problems and Multi-Parameter Models of Kinetic Fermentation, and Rheological Data

- **April Miller**, Corey James, Matthew Armstrona

Paper 373ab: Spatial and Temporal Hydrodynamic Parameters in a 0.3 m Diameter Bubble Column Using Wire Mesh Sensors and Pressure

— Dinesh V. Kalaga, Artur Zych, Masahiro Kawaji

Paper 373ac: Optimal Gas Treatment and Coal Blending for Reduced **Emissions in Power Plants**

- Lidia S. Guerras, Mariano Martín

Paper 373ae: Propylene Polymerization Process Modelling and Simulation

- Nikhil Prakash

Paper 373af: System Analysis for Energy Efficiency and Process Debottlenecking for a Sustainable Pulp and Paper Industry

— Luciana Savulescu, Hakim Ghezzaz, Bahador Bakhtiari, Serge Bedard

Paper 373ag: An Enhanced Column and Constraint Generation Method for Adaptive Robust Optimization with Non-Convex Subproblems

- Ricardo M. Lima, Antonio Conejo, Omar Knio

Paper 373ah: A Methodology for Global Sensitivity Analysis for the Operation of Distributed Energy Systems Using a Two-Stage Approach

- Ishanki De Mel, Evgenia Mechleri, Panagiotis Demis, Bogdan Dorneanu, Oleksiy V. Klymenko, Harvey Arellano-Garcia

Paper 373ai: A Blockchain Model for Residential Distributed Energy Resources Networks

- Evgenia Mechleri, Zarif Shafiei, Bogdan Dorneanu, Harvey Arellano-Garcia

Paper 373aj: Global Optimization for Chance-Constrained Nonlinear Programs and Its Application on the Gasoline Blending Problem

- Yu Yang, Loren dela Rosa

Paper 373ak: Optimisation of Decarbonisation Pathways for Heat and Power Sectors in the UK

- Vassilis M. Charitopoulos, Chi Kong Chyong, David Reiner

Paper 373al: Grid Edge Modernization Opportunities for Distributed Energy Resources Using Blockchain

- David M. King

Paper 373am: Thermodynamic Analysis of Hydrogen Refueling Station

- **Byungchan Jung**, Youngsub Lim

Paper 373an: Precision Healthcare Supply Chain Design Optimization Based on Trade-Off between Time and Cost

— Apoorva Katragadda, Xiaonan Wang, Iftekhar A. Karimi

Paper 373ao: Quantifying the Effects of Disruptions in LNG Supply Chains through Agent-Based Dynamic Simulation

— **Ramanan SV**, Rajagopalan Srinivasan

Paper 373ap: Procurement of LNG Under Supply and Demand Uncertainties: Portfolio Optimisation Studies

— **Mohd Shahrukh**, Rajagopalan Srinivasan

Paper 373aq: Enhancing Productivity of Multi-Process Production System By Machine Combination Optimization — Yoshiaki Suzuki**, Manabu Kano**

Paper 373ar: Simultaneous Berth and Yard Allocation Planning of Container Vessels for Port Throughput

Maximization

— **Jialin Xu**, Thomas C. Ho, Qiang Xu

Paper 373as: On the Interaction and Integration of Production Planning and (Advanced) Process Control - Omar S. Santander. Michael

Baldea, Christopher Betts Paper 373at: A Cluster-Based Strategy to Integrate the Operational Management of Crude Oil Supply

— **Leonardo Salsano de Assis**, Brenno C. Menezes, Eduardo Camponogara

Paper 373au: Coping with Severe Feed Pressure Fluctuation in Ethylene Plant Using APC & RTO

- Ahmed Al-Khatib, Firmin Butoyi, Rashed Al-Zahrani

Paper 373av: Real-Time Optimization of an Oil Refinery Heat Exchanger Network - Cesar S. Ikarimoto, Galo A. C. Le Roux

(374) Poster Session: Bioseparations Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency

Ballroom R/S Heather C. S. Chenette, Chair Pratik U. Joshi, Co-Chair

Sponsored by: Bio Separations

Paper 374a: Utilizing Gel Electrophoresis to Separate Aggreate after Photo-Crosslined Proteins – Christa N. Hestekin**, Haley Duncan**, **Gram Booth**

Paper 374b: Pilot-Scale Design of **Downstream Processing for Viral** Therapeutics Using Aqueous Two-Phase Systems

- Dylan G. Turpeinen, Pratik U. Joshi, Cameron Miller, Caryn L. Heldt

Paper 374c: Optimization of Hydrodistillation Extraction Process of Tea Tree Oil Using Response Surface Methodology

- Yen-Ju Chen, Jung-Hsuan Chou, Bing-Hung Chen, Duu-Jong Lee

Paper 374d: Magnetic Separation of Apoptotic Red Blood Cells for Better **Blood Transfusion Practices**

- James Kim, Mitchell Weigand, Jeffrey J. Chalmers

Paper 374e: Isolation and Purification of Biosurfactant Mannosylerythritol Lipids from Fermentation Broth with Methanol/ Water/N-Hexane

- Xuwei Long

Paper 374f: Optimizing the Separation of Oleanolic and Ursolic Acids by Simulated Moving Bed Chromatography using a C_{30} Adsorbent

– Ivo S. Azenha**, Jose P. S. Aniceto**, Adélio Mendes, Carlos M. Silva

(375) Poster Session: Chemical **Engineering Education**

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Daniel Lepek, Chair Alex J. Bertuccio, Co-Chair

Sponsored by: Education

Paper 375a: Reading Analytics and Cramming Using an Interactive Textbook for Material and Energy Balances

- Matthew Liberatore

Paper 375b: Improving a Graduate Pedagogy Course to Support Inclusive Teaching and Active Learning - Shannon Ciston, Kara Fong

Paper 375c: It's Electric! Incorporating Battery Experiments into Senior Unit Operations

Alex J. Bertuccio, Brittany Graber

Paper 375d: Strategies for Handson Activities Integrated in an Undergraduate Engineering Curriculum — Huy Pham, Cerasela Zoica Dinu

Paper 375e: Design of an Open-Ended Unit Operations Experiment in Transport Phenomena

— Joe Chada

Paper 375f: Use of Business Model Canvas in Bioprocesses Engineering Education at Undergraduation Level: Encouraging Entrepreneurship and Increasing Motivation

- Ângela Maria Moraes, Monize Caiado Decarli, Cecília Buzatto Westin, Marco César Prado Soares, Franciele Flores Vit. Fernan David Martinez Jimenez, Lucimara Gaziola de Latorre

Paper 375g: Laying a Foundation with Outcome Assessment in Material and **Energy Balances**

— Christy Wheeler West

Paper 375h: Integrating VBA-Excel into the Curriculum across Seven Junior-Year

- Kevin N. West, Christy Wheeler West, Brooks D. Rabideau

Paper 375i: Fair or Foul – Food Freshness Beyond the Smell Test — James P. Abulencia, Aravind Suresh

Paper 375j: Unit Conversions Meet Google Analytics: Insights into How Chemical Engineers Use Mobile Apps — Jason E. Bara

Paper 375k: Homework Problem Repository and Delivery System for Quantitative Problems

— **John Wagner**, Amanda P. Malefyt, James Canino

Paper 3751: Simview VR: a Software Pipeline for Virtual Reality Real-Time Molecular Dynamics Simulation and Visualization of Arbitrary Molecules — Heta Gandhi, Rainier Barrett, Andrew White

Paper 375m: Predicting Success in Undergraduate Chemical Engineering at the United States Military Academy

— Trevor Corrigan

Paper 375n: A Look into How Students Take up Realistic Instructional Tasks — *Milo D. Koretsky*, *Edward L. Michor*, Susan Nolen

Paper 375o: An Interdisciplinary Research Site for Emerging Researchers within the Functional Materials and Manufacturing Institute at University of South Florida

— **John N. Kuhn**, Venkat R. Bhethanabotla, Scott W. Campbell

Paper 375p: Developing an Undergraduate Research Opportunities Programme (UROP) to Improve Students' Professional and Research Skills

— Sarah Hedberg

Paper 375q: Resource Development Approach for Enhancing Enabling Environments within Experiential Learning Modules

— **Umang V. Shah**, Pavan Inguva, Clemens Brechtelsbauer

(376) Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Sapna Sarupria, Chair Andrew Ferguson, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

Paper 376a: How Molecular Simulations Can Inform Business Decisions in Different Industrial Sectors: The Composelector Example

— Erik Laurini, Domenico Marson, Andrea Mio, Sabrina Pricl**, Maurizio Fermealia**

Paper 376b: A Machine Learning Guided Approach for Studying Local Solvation Environments

— Yasemin Basdogan, John A. Keith

Paper 376c: Relating Segregation Behavior in Metal Alloy Nano-Particles of Different Shapes and Sizes

— Gargi Agrahari, Abhijit Chatterjee

Paper 376d: Influence of Composition on Nucleation Process in CuNi System — Solène Bechelli, Brittany Gonzalez, Caroline Desgranges, Jerome

Delhommelle

Paper 376e: Automating Transferable Coarse-Model Generation and Back-Mapping with an Open Source Toolchain — Michael Henry, Eric Jankowski

Paper 376f: Computational Study of Liposome Formation in Coaxial Turbulent Jet Flow Using CG-MD and CFD Approaches

— **Hossein Mohammadiarani**, Antonio Costa, Xiaoming Xu, Celia N. Cruz, Su-Lin Lee, Diane Burgess, Bodhisattwa Chaudhuri

Paper 376g: Analyzing the Bandgap of 3D Perovskite Oxides: Machine Learning Approach

— **Robert Kuramshin**, Omar Allam, Seung Soon Jang

Paper 376h: Investigating Hybrid Organic-Inorganic Tin Perovskites for Li-Ion Battery Applications: DFT Modeling Approach

— **Jihoon Kim**, Omar Allam, Seung Soon Jang, Jiankun Pu

Paper 376i: Statistical Learning Approaches for Identifying Descriptors of Metal/Support Interactions in Catalysis

— **Chun-Yen Liu**, Shijia Zhang, Meng Li, Thomas P. Senftle

Paper 376j: Multi-Scale Simulations with Linear Scaling Relations and Microkinetic Models of Aqueous Phase Reforming of Sugar Alcohols

— **Tianjun Xie**, Rachel B. Getman

Paper 376l: DNA Adsorption on Graphene: DFT Modeling Approach

— Vaibhav Vasudevan, Dong Gun Oh, Ha Young Hwang, Seung Soon Jang

Paper 376m: Multiscale Modeling of the UV-Sensitive Spiropyran/Merocyanine Micelles

— **Mackenzie Mallard**, SeungMin Lee, Connor Callaway, Seung Soon Jang

Paper 376n: Artificial Neural Networks for Accurate Prediction and Analysis of Perovskite Bandgaps

— **Zlatomir Stoichev**, Omar Allam, Seung Soon Jang

Paper 376o: First-Principles Study on Developing Li₁₀-XSnP₂S₁₂-XCl₂ Electrolyte with Outstanding Li-lon Conductivity for High-Voltage Solid State Batteries

— **Kyungju Nam**, Jeemin Hwang, Byungchan Han

Paper 376p: First-Principles Study on Unexpectedly Large Lattice Expansion of PdHx Nanoparticles Generated in Situ in TEM Graphene Liquid Cell

— **SungJun Hong**, Hoje Chun, Byungchan Han Paper 376q: Structure and Gas Transport Properties of Organic Mixed Matrices: Polymers of Intrinsic Microporosity with Organic Molecules of Intrinsic Microporosity

— **Alexander Demidov**, Ping Lin, Coray M. Colina

Paper 376r: Transport Mechanisms of Polar Solutes in a Cross-Linked Hii Phase Lyotropic Liquid Crystal Membrane

— **Benjamin J. Coscia**, Michael R. Shirts

Paper 376s: Towards Rational Design of Chemical Modulators to Improve Plant Drought Tolerance

— Chuankai Zhao, Diwakar Shukla

Paper 376t: Rosette Nanotubes for Applications in Water Filtration, Biosensing and Drug Delivery: A Molecule Dynamics Study

— **Vyshnavi Karra**, Prabhat Tirpathi, Meni Wanunu, Sidi Bencherif, Hicham Fenniri, Francisco R. Hung

Paper 376u: Investigating the Core-Shell Structure of Soot Using Molecular Modelling Methods

— **Kimberly Bowal**, Jacob W Martin, Peter Grancic, Markus Kraft

Paper 376v: Atomistic Simulation Studies of Artificial Water Channels in Membranes

- Yong Liu, Harish Vashisth

Paper 376w: Deciphering the Effects of a Triple Mutation on the Structure and Dynamics of Human Interferon Alpha 2-a Via Atomistic Simulations

— **B. Lakshitha A. Perera**, Ping Lin, Coray M. Colina

Paper 376x: Molecular Dynamics Simulations of New Ionic Liquids with Crystal-like Structures As Highly Selective Membrane Materials for CO₂ Separation

— **Xiaoyang Liu**, Kathryn E. O'Harra, Jason E. Bara, C. Heath Turner

Paper 376y: Prediction of Rheological Properties of Ldpe Produced in High-Pressure Tubular Reactors

— **Maira Dietrich**, Mariano Asteasuain, Adriana Brandolin, Claudia Sarmoria

Paper 376z: Development of a New Computational Tool to Study Protein Assembly at the Blood-Brain Barrier Interface

— **Nandhini Rajagopal**, Shikha Nangia

Paper 376aa: A Bayesian Approach to Model Selection and Parameterization for Non-Bonded Interactions

— **Owen Madin**, Richard A. Messerly, Michael R. Shirts

Paper 376ab: Modulating Protein Conformational Dynamics Via Salt-Bridging Interactions

— **Mohammadjavad Mohammadi**, Harish Vashisth

Paper 376ac: The Use of Experiment Directed Simulations to Improve the Accuracy of Simulations

— **Dilnoza Amirkulova**, Maghesree Chakraborty Paper 376ad: Developing First-Principles Based Interatomic Potentials with Bayesian Inference

- Noushin Omidvar, Hongliang Xin

Paper 376ae: Free Energy Calculation on Human β Defensin Type 1 in Different Redox Conditions

- Rabeta Yeasmin, Liqun Zhang

Paper 376af: Molecular Dynamics
Simulation on Human Beta-Defensin
Type 3 Binding with CXCR₄ Receptor
— Jackson S. Penfield, Ligun Zhang

Paper 376ag: Atomistic Insight Toward Dynamic Interactions in Pegylated Bovine Serum Albumin

— **Aravinda Munasinghe**, Akshay Mathavan, Akash Mathavan, Ping Lin, Coray M. Colina

Paper 376ah: Molecular Dynamics Modeling Based Investigation of Cryoconcentration of Solutes during Freezing and Its Impact on Protein Stability

— **Tibo Duran**, Bruna Minatovicz, Hossein Mohammadiarani, Bodhisattwa Chaudhuri

Paper 376ai: High-Pressure
Phenomena in Adsorbed Films: A New
Route to an Experimental Determination
of Effective Tangential Pressure
— Kaihang Shi, Erik E. Santiso, Keith

Paper 376aj: Applications of *Freud* for Nanoscale Simulation Analysis

— *Vyas Ramasubramani*, *Bradley Dice*, *Eric S. Harper, Matthew Spellings*,

Joshua A. Anderson, Sharon C. Glotzer

F Gubbins

Paper 376ak: Building Computational Tools to Help Guide Experimentalists in the Discovery of New Solid Phases of Organic Materials

- Nathan Abraham, Michael R. Shirts

Paper 376al: Metal Organic
Frameworks As Cargos for the Delivery
of an Anti-Cancer Drug, Curcumin
— Abhishek Sose, Samrendra Singh,
Yaxin An. Sanket A. Deshmukh

Paper 376am: Foyer: A Framework for Defining Force Field Usage Semantics and Atom-Typing Molecular Systems

— Justin Gilmer, Christoph Klein, Andrew Z. Summers, Matt Thompson, Peter T. Cummings, Clare McCabe, Peter Volgyesi, János Sallai, Christopher R. Iacovella

Paper 376an: Electrochemical Reduction of CO₂ on Transition Metal- P Block Compositions

— **Sahithi Ananthaneni**, Rees B. Rankin

Paper 376ao: Melting of Glucose Disaccharides Using Molecular Dynamic Methods

— **Eboni Hobley**, Vinayak N. Kabadi

Paper 376ap: Systematic Coarse-Grained Mapping and Potential Learning — Maghesree Chakraborty, Andrew White Paper 376aq: Phase Thermodynamics and Ab Initio Simulations to Optimize Oxidation Resistance of High Entropy Alloys in Additive Manufacturing

— Zachary Ulissi, Amish Chovatiya, Bryan Webler, Yining He, Maarten De

Paper 376ar: Mosdef: A Python-Based Molecular Simulation and Design Framework

Boer, Jose Loli

— Justin Gilmer, Christoph Klein, Matthew W. Thompson, János Sallai, Andrew Z. Summers, Christopher R. Iacovella, Ákos Lédeczi, Peter Volgyesi, Clare McCabe, Peter T. Cummings

Paper 376as: Modeling Inhibition of Biocatalysts By Ionic Liquids Using Metadynamics

- Sarah Alamdari, Jim Pfaendtner

Paper 376at: Automated Implementation of Trappe Force Fields Using Mosdef

— **Becky Eggimann**, Colin Bunner, J. Ilja Siepmann

Paper 376au: An Accurate Coarse-Grained Model of Poly(acrylic acid) with Explicit Solvent Models of DMF and Water

— **Yaxin An**, Samrendra Singh, Karteek K. Bejagam, Sanket Deshmukh

Paper 376av: Mechanistic Insights into Electrolyte Stability Toward Li/Na Anodes

- Xiang Chen, Qiang Zhang

Paper 376aw: The Transport
Mechanism of CO₂/CH₄ Mixtures in Ionic
Polyimides and Ionic Liquid Composite
Membranes – MD Simulation Studies

— Joanna Szala-Bilnik, **Henry Atkinson**, Asghar Abedini, Jason E. Bara, C. Heath Turner

Paper 376ax: Understanding Temperature-Induced Self-Folding of Thermo-Sensitive Polymer Grafted Graphene

— Karteek K. Bejagam, Samrendra Singh, **Soumil Y. Joshi**, Sanket A. Deshmukh

Paper 376ay: Elucidating Biofuel Sooting Mechanisms: A Combined Reaxff and DFT Study

— **Richard A. Messerly**, Brian Etz, Hyunguk Kwon

Paper 376az: Molecular Dynamics Simulation on Interaction of Human Beta Defensin Type 3 with Different Lipid Bilayers

— Mouhmad Elayyan, George Rucker, Yilun Lee, Rabeta Yeasmin, **Liqun Zhang**

Paper 376ba: Simulation Study of Macromolecules Propagation Mechanism in Heterogeneous Porous Media

— **Jianqiao Leng**, Yang Zhao, Baojun Bai, Mingzhen Wei

Paper 376bb: Protein Corona on a Gold Nanoparticle Studied with Discontinuous Molecular Dynamics and Atomistic Molecular Dynamics Simulations

— Size Zheng, Ying Wei, Chidumebi Alim, Eliel Akinbami**, Md Symon Jahan Sajib**, Tao Wei Paper 376bc: On the Phase Behavior of Water like Fluid Models in Slit-like Pores with Walls Covered By Molecular Brushes

— **Victor Trejos**, Orest Pizio, Stefan Sokolowski

Paper 376bd: Wetting Behavior of Imidazolium Based Ionic Liquids: A Molecular Dynamics Study

— **Sandip Khan**, Sanchari Bhattachariee

Paper 376be: First Principles-Based Multiscale Atomistic Methods for Next-Generation Electrocatalysts

— Saber Naserifar

Paper 376bf: Development of a Generic Mathematical Optimization-Based Nanomaterial Design Toolkit

— **Christopher L. Hanselman**, David C. Miller, Chrysanthos E. Gounaris

Paper 376bg: Modelling Micellization of Rhamnolipid Biosurfactant By Mesoscale Simulation

— Zong-Yuan Cai, Yun-Chung Pan, **Ming-Tsung Lee**

Paper 376bh: Oxidation State of Solutes in Molten Salts from Ab Initio Molecular Dynamics Simulations

- Austin Clark, Stella D. Nickerson

Paper 376bi: Quantum-Based Predictions for Network-Altering Chemical Reactions in Siloxane Polymer Systems

— **Matthew P. Kroonblawd**, Nir Goldman, James Lewicki

Paper 376bj: Computational Corrections for Long Range Interactions in Periodic Simulations

— Sahar Zenoozi, Jakin B. Delony, Clifford L. Henderson, **Peter J. Ludovice**

Paper 376bk: Mixed-Metal Influence on Purity of Process Performance for Metal-Organic Frameworks with Open Metal Sites for Olefin/Paraffin Separation

— **Wenqin You**, Trisha Sen, Matthew J. Realff, David S. Sholl

Paper 376bn: Design and Analysis of High-Spin Ground State Donor-Acceptor (DA) Polymers: A Computational Study

— **Md Abdus Sabuj**, Md Masrul Huda, Neeraj Rai

Paper 376bo: Stability of Ligand Protected Au Nanoclusters Under Electrochemical Reduction of CO₂

— Anantha Venkataraman Nagarajan, Rosalba Juarez-Mosqueda, Michael Cowan, Giannis Mpourmpakis

Paper 376bp: Energy Profiles of the Ring Puckering of Cyclopentane, Methylcyclopentane and

Ethylcyclopentane

— Martin R. Schenk, Karl N. Kirschner, Steven M. Graham, Wolfgang Heiden, Dirk Reith

Paper 376bq: Effects of Coexisting Familial Mutants on Wild Type Amyloidβ21-30 Assembly

— **Maghesree Chakraborty**, Heta Gandhi, Dilnoza Amirkulova, Andrew White Paper 376br: Studying Shape-Dependence of Structural Conformations for Coarse-Grained Thermo-Sensitive Bottle-Brush Polymer Models

— **Soumil Y. Joshi**, Karteek K. Bejagam, Yaxin An, Sanket A. Deshmukh

Paper 376bs: Computational Studies of the Oxidation and Reduction of Pd-Ag Alloy

— Kaining Duanmu, Christopher O'Connor, Cynthia M. Friend, Phillippe Sautet

Paper 376bt: Contacts between
Molecular Surfaces Allow Quick
First-Principle Prediction of Dielectric
Constant in Pure Liquids and Mixtures
— Théophile Gaudin, Haibo Ma

Paper 376bv: Efficient Generation of Full-Atomistic Polymer Amorphous Structure Adsorbed onto Solid Surfaces by Reverse-Mapping technique

— **Hiroya Nitta**, Taku Ozawa

(377) Poster Session: Fundamentals and Applications of Adsorption and Ion Exchange

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Aaron Moran, Co-Chair

Sponsored by: Adsorption and Ion Exchange

Paper 377a: Adsorption of Amoxicillin in Contaminated Water from Canebagasse Ash

— Juan D. Alonso, Juan S. Lopez, Yuby Cruz, Francisco Rodriguez, Idoia Estiati, Juan F. Saldarriaga Sr.

Paper 377b: Incorporating a Vacuum Pump Performance Curve in Cyclic Adsorption Process Simulation

— **Huan Jiang**, Armin D. Ebner, James A. Ritter

Paper 377c: Process Simulation of Removal Methyl Sulfide from Nitrogen Using Pressure Swing Adsorption Based on Aspen Adsorption

— **Yonghou Xiao**, Mingpu Yuan, Shuang Qiu, Gaohong He

Paper 377d: Evaluation and Optimization of Vpsa Processes with Nanostructured Zeolite NaX for Post-Combustion CO, Capture

— **Mai Xu**, Shaojiang Chen, Dong-Kyun Seo, Shuguang Deng

Paper 377e: A Novel CO₂ Capture Process with High Flexibility and Productivity

— Yixuan Zhang, Hyungwoong Ahn

Paper 377f: Flexible MOFs for Gas Separation – a Case Study Based on Static and Dynamic Sorption Experiments

— Christian Reichenbach, Andreas Möller, Robert Eschrich, Jens Möllmer, Marcus Lange, Hannes Preißler, Roger Gläser

Paper 377g: Computational Modelling of CO₂ and CH₄ Diffusion in Bulk ZIF-8

— Hari Paudel

Paper 377h: Adsorption Kinetics of CO₂ By Amine Groups

- Mohammed S. Ba-Shammakh

Paper 377i: Single and Binary Component Adsorption of 1-Alcohols from an Alkane Using Various Activated Alumina Adsorbents

— **Cara E. Schwarz**, Catherine E. Bosman

Paper 377j: Chitosan Functionalized with Histidine to Increase Metal Ions Adsorption

- Rodrigo Silveira Vieira

Paper 377k: Successful Recovery and Concentration of 5-Hydroxymethylfurfural from Aqueous Solutions Onto Various Polymeric Adsorbent with Different Functional Groups

— Jiayi Zheng, Jiangxiong Xiao, Xianda He, Zhe Chen, Baoying Pan, Yao Liu, Xiaojie Zheng, **Xiaoqing Lin**

Paper 377I: Development of Highly Selective Composite Adsorbents for Selective Recovery of Gold (Au³*) and Silver (Ag+) Ions from Electronic Wastes (E-wastes)

— **Hiluf Tekle Fissaha**, Khino J. Parohinog, Lawrence A. Limjuco, Grace M. Nisola, Wook-Jin Chung

Paper 377m: High Vying Ti₃C₂Tx Mxene Nanosheets with Mehpa to Release Mercury from a Loaded Oil Phase

— **Saeed Laki**, Ahmad Arabi Shamsabadi, Farbod Alimohammadi, Babak Anasori, Masoud Soroush

Paper 377n: Capture of Alkynes from Hydrocarbon Mixtures with Multi-Functional Metal-Organic Framework By Combining Molecular Recognition and Size-Sieving

— **Qingju Wang**, Xili Cui, Zhaoqiang Zhang, Lifeng Yang, Huabin Xing

Paper 377o: An Alternative Synthetic Method for Porous Organic Cage CC₃ in Dimethylformamide

— **Jolie Lucero**, James M. Crawford, Carla Osuna. Moises A. Carreon

Paper 377p: Study of Lanthanum Carbonate Modified Microfibrous Composite for Phosphate Adsorption in Wastewater

— Yi Yang, Kok Yuen Koh, **J Paul Chen**, Huiping Zhang

Paper 377q: Room-Temperature Synthesis of Carboxylated-Mxene Nanosheets for Mercury Scavenging — Saeed Laki, Ahmad Arabi

— **Saeed Laki**, Ahmad Arabi Shamsabadi, Farbod Alimohammadi, Babak Anasori, Masoud Soroush

Paper 377r: A Novel Glycine-Modified Cu-BTC with High Capacity and Enhanced Stability for Efficient Separation of C₂H₆and C₂H₄ — Yufang Wu, Xin Zhou, Jing Xiao, Zhong Li

Paper 377s: A Comparison of Gas Adsorption Capacities of Isostructural Metal Organic Frameworks: [[Cu₂(abtc)]₃] Versus [[Cu₂(reduced abtc)₃]

— **Prudhviraj Medikonda**, Sastri Chivuluka, Sasidhar Gumma Paper 377t: Electrochemical Synthesis of Ammonia, and Development of Nanoporous Carbon-Composite Adsorbent Exhibiting High Ammonia Uptake — Kanghee Cho, Hyung Chul Yoon, Hee-Tae Beum, Sun Hyung Kim, Jong-Nam Kim

Paper 377u: Green and Sustainable Chromatographic Separation Strategy for Levulinic Acid from Biomass Hydrolysate

— Xiaoqing Lin, KeXuan Zhang, Jiayi Zheng, Yao Liu, Xiaojie Zheng, Jiangxiong Xiao, Xianda He

Paper 377v: Propane-Selective Adsorbent g-C₃N₄@Zr-BPDC for Efficient Propylene Purification

- Xin Zhou, Sa Wang

Paper 377x: Transport Kinetics and Selectivity for Carbon Dioxide and Water for Gas Phase Electrolysis

— **Nicholas R. Schwartz**, Philip Cox, Jason Harrington

Paper 377y: Using Lithium-Aluminum Layered Hydroxide As an Efficient Adsorbent to Recover Lithium from Brine — Jing Zhong, Sen Lin, Jianguo Yu

Paper 377z: MOF-GO Hybrid Nanocomposite Adsorbents for Methane Storage — Qasim Al-Naddaf, Mana Al-Manssour. Fateme Rezaei

(378) Poster Session: General Topics on Separations

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Joshua A. Thompson, Chair Stephen M. Ritchie, Co-Chair

Sponsored by: General Topics and Other Methods

Paper 378a: Two-Dimensional-Material Mixed-Matrix Membranes for Gas Separation

— Jie Shen**, Gongping Liu**, Wanqin Jin

Paper 378b: Development of the Novel Manufacturing Process of High Purity LiOH • H₂O from Li₂CO₃ Using Acetic Acid — Akinori Jonoshita, Hideki Yanganto Sr.

Paper 378d: Ionic Transport in Reverse Osmosis Membrane

— Tianyu Chen

Paper 378e: Butene Oligomerization within Dividing Wall Column

— **Huidian Ding**, Qiang Li, Wanbo Li, Zhihai Zhao, Changzhi Shi

Paper 378f: Enhancement of Baffles with Different Sizes and Intervals on Mass Transfer in Microchannels

— **Yaran Yin**, Daofan Ma, Chunying Zhu, Taotao Fu, Xiqun Gao, Youguang Ma

Paper 378g: Solubility of L-Phosphinothricin and Its Hydrochloride in Water + (Methanol, Ethanol) Binary Solvent Mixtures from 278.15 K to 318.15 K — Yayun Liu, Shuyun Ju, Jianping Wu, Gang Xu, Lirong Yang $\begin{array}{ll} \textbf{Paper 378h:} \ \textbf{H}_2 \ \textbf{Membrane Separation} \\ \textbf{and} \ \textbf{C}_3 \textbf{H}_8 \ \textbf{Vaporization Synergistic} \\ \textbf{for Energy Saving in Oleflex} \\ \textbf{Dehydrogenation Process} \end{array}$

— Xuehua Ruan, Hongyan Xiao, Gaohong He, Xiaobin Jiang

Paper 378i: Development of Acoustic-Driven Packing Material a Novel Uky-Caer Technology for CO₂ Capture — Bradley Irvin, Heather Nikolic, Kunlei Liu

Paper 378j: Distillation Performance in Packed Columns with Structured Packing: Numerical Simulation Considering the Liquid Distribution Profiles

— **Kazutoshi Ishizaki**, Hitoshi Kihara, Nobuaki Egoshi

Paper 378k: Composition and Temperature Cascade Control with Model Predictive and PI Controllers for Dividing-Wall Distillation Columns

— **Xing Qian**, Kejin Huang, Shengkun Jia, Haisheng Chen, Yang Yuan

Paper 378I: Optimizing Fractionation Condenser System CAPEX and OPEX— Case Studies & Performance

- Eric Parvin

Paper 378m: Wash Oil Control:Inferred Versus Measured Rates

- Andrew W. Sloley

Paper 378n: Minimum Reflux Calculation for Multicomponent Azeotropic Distillation Using Shortcut Method

- Zheyu Jiang

Paper 378o: Biodiesel Separation Using Ultrafiltration Poly(ether sulfone) Hollow Fiber Membranes: Improving Biodiesel and Glycerol Rich Phases Settling

— **Mario Andrés Noriega**, Paulo César Narváez Rincón, Alberto Claudio Habert

Paper 378p: Molecular Simulations of Carbon-Based Adsorbents/Membrane Materials for Sustainable Processes

— **Daniel Bahamon**, Nour Alkhatib, Ki Ryuk Bang, Eun Seon Cho, Mohammad Abu Zahra, Maryam Khaleel, Lourdes F. Vega

Paper 378q: Model of the Multi-Channel Ceramic Membrane for so₂ Absorption — *Xiangli Kong*, *Minghui Qiu*, Fan Yiaun

Paper 378s: A Predictive Model for Seawater Reverse Osmosis Module — *Mingheng Li*

Paper 378t: Modelling Oxygen Permeation across the Membrane of an Alternative Membrane Reactor for Oxidative Coupling of Methane

— **Ojotule P Onoja**, Panagiotis Kechagiopoulos

Paper 378u: Modeling the Ion Transport and Adsorption Behavior in a Membrane Capacitive Deionization (mCDI) Cell

— Xin Zhang, Danny Reible

Paper 378v: A General Predictive Model for Comparative Study of Vacuum Membrane Distillation and Sweeping Gas Membrane Distillation

— **Amit Thakur**, I-Min Hsieh, M. R. Islam, Chau-Chyun Chen, Mahdi Malmali

Paper 378w: Design and Fabrication of High-Performance Hollow Fiber Membrane Devices for Direct Contact Membrane Distillation

— Abdullah Al Balushi, **Mahdi Mohammadi Ghaleni**, Mona Bavarian, Siamak Nejati

Paper 378x: Apply Nanocomposite Material for Hydrogen Separation and Purification

— **Qasim Al-Naddaf**, Fateme Rezaei

Paper 378y: In situ Microextraction/ Stripping Using Supported Liquid Membrane (SLM): A Comprehensive Numerical Study

— **Tao Wang**, Cong Xu

(379) Poster Session: In Recognition of the 50th Anniversary of ExxonMobil Corporate Strategic Research

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S Yogesh Joshi, Chair Sara Yacob, Co-Chair

Sponsored by: Poster Sessions

Paper 181ar: Accelerated Design of Molecular Additives for Polymer Crystallization

— **Corinne L. Carpenter**, Gregory C. Rutledge, Richard D. Braatz

Paper 563d: Study of the Influence of Antifoaming Additives on the Crude OIL/ Air Interface By Rheology

— **Mariana Mendes**, João B. V. S. Ramalho, Osvaldo Karnitz Jr., Luiz Carlos Palermo, Claudia E. Mansur

Paper 560dv: Mechanism of Oxidative Dehydrogenation of Ethane at High Temperatures

— **Hilal Ezgi Toraman**, Gerhard R. Wittreich, Dionisios G. Vlachos

Paper 560ek: Kinetics of $\rm O_2$ Activation over Cu-Exchanged Zeolites: Implications for Partial Methane Oxidation

— **Daniel T. Bregante**, Laura N. Wilcox, Rajamani Gounder, David Flaherty

Paper 381h: High-Performance Mixed-Matrix Membranes for Propylene/ Propane Separation By *in-Situ* MOF Formation Using a Polymer-Modification Strategy

— **Sunghwan Park**, Hae-Kwon Jeong

Paper 376e: Automating Transferable Coarse-Model Generation and Back-Mapping with an Open Source Toolchain — *Michael Henry, Eric Jankowski*

Paper 560bp: Influence of Coordination Environment Around Anchored Single-Site Cobalt Catalyst for CO₂ Hydrogenation

— **Juan Jimenez**, **Mi**chael Royko, Jochen Lauterbach Paper 563e: Experimental and
Theoretical Study of Viscosity Behavior
of Sulfonated Partially Hydrolyzed
Polyacrylamides (S-HPAM) with LongTerm Thermal Stability

— Xiaona Hu, Zhuo Yi, Xi Liu,

— Xiaona Hu, Zhuo Yi, Xi Liu, Lunyu Zhu, Zhao Fang, Jinbiao Yang, Yajing Li

Paper 560hd: Development of an Accelerated Deactivation Protocol for Vacuum Gasoil Hydrocracking Catalysts

— **July Carolina Vivas Báez**, Gerhard D. Pirngruber, Alberto Silva Servia, Anne-Claire Dubreuil, David de Jesús Perez Martinez

Paper 381ar: Purification of Ethylene with Anion-Pillared Metal-Organic Frameworks As Adsorbents

— **Qi Ding**, Xili Cui, Zhaoqiang Zhang, Lifeng Yang, Huabin Xing

Paper 376j: Multi-Scale Simulations with Linear Scaling Relations and Microkinetic Models of Aqueous Phase Reforming of Sugar Alcohols

— Tianjun Xie, Rachel B. Getman

Paper 181bd: Synthesizing Novel Degradable Polymers with Tunable Mechanical Properties

— Whytneigh R. Duffie, Eswar Arunkumar Kalaga, Timothy M. Brenza, Travis W. Walker

Paper 377n: Capture of Alkynes from Hydrocarbon Mixtures with Multi-Functional Metal-Organic Framework By Combining Molecular Recognition and Size-Sieving

— **Qingju Wang**, Xili Cui, Zhaoqiang Zhanq, Lifenq Yanq, Huabin Xinq

Paper 185c: Computational Analysis of MOF-Enzyme Interactions for Next Generation of Sensitive Biosensors

— **Jordan Chapman**, Nagasree Garapati, Ahmed E. Ismail, Cerasela Zoica Dinu

Paper 560gv: Rational Catalyst Design: Kinetics Put into Action for Small Open Data

— **Pedro S.F. Mendes**, Sébastien Siradze, Laura Pirro, Joris W. Thybaut

Paper 378t: Modelling Oxygen Permeation across the Membrane of an Alternative Membrane Reactor for Oxidative Coupling of Methane

— **Ojotule P Onoja**, Panagiotis Kechagiopoulos

Paper 376y: Prediction of Rheological Properties of Ldpe Produced in High-Pressure Tubular Reactors

— **Maira Dietrich**, Mariano Asteasuain, Adriana Brandolin, Claudia Sarmoria

Paper 183y: Preparation and Characterization of a Novel Electrospun Activated Carbon/Whey Protein/ Polycaprolactone Membrane for Heavy Metals Removal

— Laura Cristina Ramírez-Rodríguez, María Ximena Quintanilla Carvajal, Edisson Tello, Carlos A. Jiménez-Junca Paper 563b: The Influence of Ammonia on Flame Characteristics and Soot Formation in Ammonia/Methane **Diffusion Flames**

— **Matthew Montgomery**, Hyunguk Kwon, Yuan Xuan, Lisa Pfefferle, Charles S. McEnally

Paper 560hi: Fin-like Zeolite Catalysts: A New Class of Hierarchical Materials — **Heng Dai**, Yufeng Shen, Donglong Fu, Thuy T. Le, Taimin Yang, Matthias Filez, Xiaodong Zou, Bert M. Weckhuysen, Jeffrey D. Rimer

Paper 183ab: A Commercially-Viable One-Step Synthesis Method to Prepare MWW Zeolite Nanosheets

— Yunwen Zhou. Mina-Fena Hsieh. Bernd Kabius, Yanyu Mu, Robert Rioux, Jeffrey D. Rimer

Paper 183h: Modeling the Reactivity of Open Metal Sites in Metal Organic Frameworks for Olefin Paraffin Separation

- Lin Li, Mona H. Mohamed, Yahui Yang, Sen Zhang, Kushantha Withanage, Juan Peralta, Koblar Jackson, Götz Veser, Nathaniel L. Rosi, J. Karl Johnson

Paper 181bb: Multi-Scale Modeling of Fiber-Matrix Interphase

- Salman Zarrini, Cameron F. Abrams

(380) Poster Session: Particle **Technology Forum**

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

William A. Hendrickson, Co-Chair Michael J. Molnar, Co-Chair

Sponsored by: Particle Technology

POWDER TRIBOELECTRICS AND SAFETY

Paper 380b: Measuring Food Powders Electrical Properties as a Result of **Humidity Content**

— Naveen M. Tripathi, Filip Francqui, Thomas Pirenne, Geoffroy Lumay

Paper 380c: Solids Metrics for Successful 3D Printing of Energetic Feedstocks

- Bryan J. Ennis, Benjamin Ennis, Brandon Ennis, Naseem Jibrin

Paper 380d: Powder Permeability As a Measurement Surrogate for Triboelectric Charging

Michael Winn, Benjamin Ennis, Naseem Jibrin, Bryan J. Ennis

Paper 380e: Metal Dust Explosion Risks: A Hazard Analysis and Review of Contemporary Industry Objectives

- Nicholas Reding, Mark B. Shiflett

■ FINE POWDER NUCLEATION AND SYNTHESIS

Paper 380f: Effect of Temperature on the Structural Parameter of Graphene Oxide

Pradip Das, Sasidhar Gumma, Bishnupada Mandal

Paper 380g: Oxidation of Carbon Black Agglomerates

- Georgios A. Kelesidis, Sotiris E. **Pratsinis**

Paper 380h: Tungsten Nitride ALD Nanofilms for Reducing Hydrogen Diffusion

- Sarah Bull. Theodore Champ. Chanel Hill, Robert C. O'Brien, Charles B. Musgrave, Alan W. Weimer

Paper 380i: Plant Based Illumination **Enabled By Functionalized** Nanophosphor Particles

- Pavlo Gordiichuk, Sarah Coleman, Juyao Dong, Daichi Kozawa, Tedrick Thomas Salim Lew, Michael Strano

Paper 380j: Correlation of Structure-Property Relationship of Dry-Coated Particle for All-Solid-State Battery

Risa Sakurai, Hideya Nakamura, Shuji Ohsaki, Satoru Watano

Paper 380k: Flame Synthesis of Catalytically Active Solid Solution Catalysts for Low Temperature Methane Oxidation

- Jennifer Naglic, Nicole Cordonnier, Frdem Sasmaz

Paper 380I: Dynamics of Early Soot Formation By Reactive Molecular **Dynamics**

- Eirini Goudeli, Somesh Roy

Paper 380m: Soft-Templating Synthesis of Hollow Metal Phosphate Nanospheres

- Samira Munkaila, Bishnu P. Rastakoti

Paper 380n: Novel Closed Spiral Reactor for Supercritical Hydrothermal Synthesis of Nanoparticles

— **Arjun Kumar Pukkella**, Nagaravi Kumar Varma Nadimpalli, Sivakumar Subramanian, Venkataramana Runkana

■ CHEMICAL LOOPING COMBUSTION

Paper 380o: Chemical Looping Partial Oxidation of Methane: The Impact of Particle Size of Hematite on Syngas Selectivity

- Yan Liu, Mengqing Guo, Josh Goetze, Lang Qin, Liang-Shih Fan

Paper 380p: Exploring Particle Modification Strategies to Improve Yields for Oxidative Coupling of Methane in a Chemical Looping System

- Deven Baser, Zhuo Cheng, Sourabh Nadgouda, Lang Qin, Liang-Shih Fan

Paper 380q: Robust Perovskite Oxygen Sorbent Particles for "Low Temperature" Thermochemical Air Separation

- Emily Krzystowczyk, Jian Dou, Xijun Wana, Fanxina Li

Paper 380r: Multiscale Modeling of Group D Iron Oxide Particles in Chemical Looping Systems: From Atomisitc Scale to Continuum Scale

- Yu-Yen Chen, Sourabh Nadgouda, Mengqing Guo, Yitao Zhang, Andrew Tong, Liang-Shih Fan

Paper 380s: Design of Fluidized Bed Combustor Reactor in Chemical Looping Combustion: Hydrodynamic and Heat **Transfer Properties**

— Yitao Zhang, Jianhua Pan, Dawei Wang, Dikai Xu, Andrew Tong, Liang-

■ PARTICLE FUNCTIONALIZATION

Paper 380t: Imiquimod Particle Formation Using the Supercritical Antisolvent (SAS) Process

Paula de Freitas Rosa Remiro, Ângela Maria Moraes, Paulo de Tarso Vieira e Rosa

Paper 380u: Surface Functionalization of Polymer Latex Particles and Its Effect on in-Situ Deposition of Nano-Sized Calcium Silicate Hydrate

Guanzhi Cheng, Yifan Liu, Quanxiao Dong, Yongjiang Xie, Xinguo Zheng, Wei Deng

Paper 380v: ZnO Nanoparticles Incorporated MIL-100 for Doxorubicin Delivery

- Abhik Bhattacharjee, Mihir K. Purkait, Sasidhar Gumma

Paper 380w: Machine Learning **Determination of Resistant and Tolerant** Bacteria Growth Modes Induced By Nanoparticles

- A-Andrew Jones, David Medina, Na Yoon Kim, Gujie Mi, Caterina Bartomeu Garcia, Lorena Baranda Pellejero, Nicole Bassous, Thomas J. Webster

Paper 380x: Overcoming the Limitations of Hydrochlorothiazide Micronization Using the Precipitation with Compressed Fluid Antisolvent Process

— **Hee Jeong Park**, Tae Jun Yoon, Dong Eui Kwon, Kyungseok Yu, Geonhwan Park, Youn-Woo Lee

Paper 380y: Characterization of Nanoparticle Size Distributions and Aspect Ratio through Single-Particle Tracking and Analytical Ultracentrifugation

- Xun Gong, Minkyung Park, Dorsa Parviz, Kevin S. Silmore, Tedrick Thomas Salim Lew, Michael Strano

MIXING, RHEOLOGY, AND **GRANULATION**

Paper 380z: Numerical Modeling of Wet **Granulation Processes**

— Tomoya Baba, Hideya Nakamura, Shuji Ohsaki, Satoru Watano

Paper 380aa: Wall Friction Measurements on Free-Flowing Material at Low Normal Stresses

— Alexander Cliff, Luke Fullard, Morio Fukuoka. Clive E. Davies

Paper 380ab: Conduction and Convection Heat Transfer in a Rotary Drum Using Simulations and Experiments

– Heather N. Emady**, Manogna** Adepu

Paper 380ac: Identifying the Impact of Processing on the Physical Properties of AM Powders and Their Subsequent Reuse

- **Tim Freeman**, Katrina Brockbank, Jeffery Kenvin, Tony Thornton

Paper 380ae: Comparative Study of Mixing in a High Shear and Low Shear Blender Using Numerical Simulation

- Koyel Sen, Natasha V. Rodriguez, Carl A. Anderson, Bodhisattwa Chaudhuri

Paper 380ag: Effect of Viscosity on Liquid Penetration in the Catalyst Impregnation Process: Experiments and Simulations

- M. Silvina Tomassone. Yanavana Shen, Jiao Yang, Jing Liu, William G. **Borghard**

Paper 380ah: In-Situ SAXS Study of the Nucleation and Growth of Precipitated

- Yubai Liu, Yujun Wang

Paper 380ai: A Conceptual Model for Analyzing Particle Effects on Gas-Liquid Flows in Slurry Bubble Columns - Rongtao Zhou, Ning Yang

■ FLUIDIZATION AND GAS-SOLID **HYDRODYNAMICS**

Paper 380ak: Hydrodynamics and Mixing in a Pseudo-2D Rectangular Spouted Bed

- Ritesh Raman. Partha S. Goswami

Paper 380al: Solids Mixing Rates of Geldart a and B Powders Predicted By the Two Fluid Model

- Mohammad-Sadegh Salehi, Maryam Askarishahi, Stefan Radl

Paper 380am: Fluid-Particle Drag in Low-Reynolds-Number Bidisperse Suspensions

— Fan Duan, Xiao Chen**, Qiang Zhou**

Paper 380an: An Investigation of Gas Fluidized Bed of Flexible Fibers Using the Coupled DEM/CFD Method

– Yiyang Jiang, Zhaosheng Yu**, Yu** Guo, Carl Wassgren, Jennifer Sinclair Curtis

Paper 380ao: Exploring Agglomerate Dynamics through an Immiscible Two-Fluid Model

- Julia Hartia, Alan W. Weimer

Paper 380ap: Using a Powder Rheometer to Probe the Defluidization of Cohesive (Group C) Particles

- Ipsita Mishra, Peiyuan Liu, Christine M. Hrenva

Paper 380aq: Fluidization of Nanopowders: Effects of Vibration and Stirring

- Fuweng Zhang, J. Ruud van

Paper 380ar: Gas-Solid Hydrodynamics and Hysteresis in a Rectangular Spouted

- Ritesh Raman, Partha S. Goswami

Paper 380as: Experimental and Simulation Study on Bubbling Behaviour of Geldart Group B Particle Pulsed Fluidized Bed

— **Ali Akhavan**, Rosemary Clark, J. Ruud van Ommen, Marc-Olivier Coppens, Martin Rhodes

Paper 380bc: Improving CO₂ Capture Efficiency in a Fluidized Bed of TiO₂ Nanoparticles

- Keju An, Jean M. Andino

■ GASIFICATION, PYROLYSIS, AND TREATMENT METHODS

Paper 380at: Computational Study on Biomass Fast Pyrolysis: Hydrodynamic Effects in a Laboratory-Scale Fluidized Bed

— Emilio Ramirez, Tingwen Li, Charles E. A. Finney, Mehrdad Shahnam, C. Stuart Daw

Paper 380au: Numerical Verification and Validation of the Biomass Pyrolysis and Gasification inside a Bench Scale Reactor with Mfix-TFM

— **Yupeng Xu**, Mehrdad Shahnam, Andrea Porcu, Alberto Pettinau, Bhima Sastri, William A. Rogers

Paper 380av: CFD Simulations of Integrated Waste Treatment Unit

— Yong Liu, Chris Guenther

Paper 380aw: Single Bubble Dynamics in a Dense Phase Fluidized Bed Gasification Environment in Presence of Biomass Pellets

— **Nicolás Torres Brauer**, Hugo de Lasa

SIMULATION AND COMPUTATIONAL TECHNIQUES

Paper 380az: Mfix-Exa: Adapting CFD-DEM to Exascale Computing

— **Madhava Syamlal**, Jordan Musser, Ann Almgren, John Bell, Christine M. Hrenya, Thomas Hauser, Peiyuan Liu

Paper 380bb: A Penalization Method for the Direct Numerical Simulation of Weakly Compressible Reacting Gas-Solid Flows

— **Baptiste Hardy**, Juray De Wilde, Grégoire Winckelmans

Paper 6cm: Finite Element Method (FEM) Modeling of Hopper Flow — Kunal S. Pardikar, Carl R. Wassgren, Chen Mao, Ariel Muliadi

(381) Poster Session: Separations Division

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Marcus Mello, Chair Roger D. Whitley, Co-Chair

Sponsored by: Separations Division

Paper 381a: Isolation Development of Co-Crystal API

— **Joe Gao**, Bing-Shiou Yang

Paper 381b: Polymer-Zeolite Dense Mixed-Matrix Membrane for Carbon-Dioxide Separation

Dragutin Nedeljkovic

Paper 381c: Separation Applications of Reduced Graphene Oxide Membranes

— **Ashish Aher**, Dibakar Bhattacharyya, Rupam Sarma

Paper 381d: Crude Oil Distillation:General Heat Integration Considerations

- Andrew W. Sloley

Paper 381e: Determination of the Effective Impurity Distribution Coefficient for Stripping Crystallization of R-2-Amino-1-Phenylethanol from the Enantiomers

- Lie-Ding Shiau

Paper 381f: Nineteen-Bore Hollow Fiber Membranes Fabrication and Applications in Oxygen Separation and Membrane Reactor

— Guangru Zhang

Paper 381g: Ultrafiltration of Colloidal Silica

— **Ikenna H. Ozofor**, Samuel D. Jacobs, Andre R. Da Costa

Paper 381h: High-Performance Mixed-Matrix Membranes for Propylene/ Propane Separation By *in-Situ* MOF Formation Using a Polymer-Modification Strategy

- Sunghwan Park, Hae-Kwon Jeong

Paper 381i: Separation of NdFeB Scrap Powder from Hard Disk Drive By HD Process

— **Chul-Joo Kim**, Kyeong Woo Chung, Ho-Sung Yoon

Paper 381j: Molecular Transport of Aqueous Mixtures in Sulfonated Polyether-Based Ion Exchange Membrane

— **Jung Min (Luca) Kim**, Breanna M. Dobyns, Bryan S. Beckingham

Paper 381k: Surface Functionalization of Magnetite for Selective Recovery of Dysprosium (Dy+3) from Permanent Magnet Waste

— **Daniel N. Mengesha**, Grace M. Nisola, Khino J. Parohinog, Hiluf Tekle Fissaha, Lawrence A. Limjuco, Wook-Jin Chunq

— **Kai Chen**, Witopo Salim, Yang Han, Michael Gasda, W.S. Winston Ho

Paper 381m: CO₂-Selective Facilitated Transport Membrane for Carbon Capture: Module Fabrication and Scale-up

— **Kai Chen**, Witopo Salim, Yang Han, Dongzhu Wu, W.S. Winston Ho

Paper 381n: Silicene As a Novel Nanofiller for Thin Film Nanocomposite Forward Osmosis Membrane

— **Anelyn Bendoy**, Hana G. Zeweldi, Wook-Jin Chung, Grace M. Nisola Paper 381o: Co(II) Recovery from Electronic Waste Based on Ion-Imprinting of Reduced Schiff Base Ligand on Magnetite

— John Edward L. Sio, Grace M. Nisola, Rosemarie Ann I. Cuevas, Khino J. Parohinog, Hiluf Tekle Fissaha, Lawrence A. Limjuco, Seong-Poong Lee, Rey Eliseo C. Torrejos, Wook-Jin Chung

Paper 381p: Application of Micropatterned and Chemically Modified PVDF Membranes for the Treatment of Produced Water Via Membrane Distillation

— **Shahriar Habib**, Steven T. Weinman

Paper 381q: Selective Separation of Rare Earth Elements from NdFeB Powders By Caustic Digestion

— **Ho-Sung Yoon**, Kyeong Woo Chung, Chul-Joo Kim

Paper 381r: Experimental and Theoretical Characterization of Thiacrown Ether Epoxy-Polymer Adsorbents for the Selective Recovery of Pd and Pt from Spent Auto-Catalyst Leachate

— **Rey Eliseo C. Torrejos**, Grace M. Nisola, Hiluf Tekle Fissaha, Khino J. Parohinog, Sang Hoon Min, Jeong Woo Han, Wook-Jin Chung

Paper 381s: Preparation and Application of Ceramic-Supported Metal-Organic Framework Membranes — Kang Huang

Paper 381t: Research Concept for the Development of Novel Additively Manufactured Structured Packings — Andreas Lange, Georg Fieg

Paper 381u: Polymer Composite Membranes Containing UiO-66 MOFs with Co-Continuously Segregated Structures for CO₂-Related Gas Separations

— **Li-Cheng Jheng**, Jaesung Park, Heewook Yoon

Paper 381v: Industrial Scale Liquid Chromatography Simulation: Separation of Cannabinoids Utilizing Different Chromatographic Technologies

— **Greg DiCosola**, Matt Zandi, Bernardo Flores, Dan Parker

Paper 381w: Design of Process Control Schemes and Experimental Investigation for a Transesterification in a Reactive Dividing Wall Column

— Lisa Egger, **Laura-Selin Harding**, Georg Fieg

Paper 381x: Physicochemical and Thermodynamic Property Determination & Modeling of Aqueous 3-Aminoproyl Triethoxysilane+Mdea/DEA within the Temperature Range of (298.15 to 333.15) K

— Sweta Balchandani, **Bishnupada Mandal**, Arvind Kumar, Swapnil Dharaskar

Paper 381y: Microscopic Diffusion of Organic Molecules in Perfluorosulfonic Acid Polymer Membranes

— **Samuel Berens**, Anastasios Angelopoulos, Sergey Vasenkov Paper 381z: In Situ Measurement of Concentration Polarization in Pressure Driven Membrane Systems Using Laser-Based Spectrophotometric Method

– **Ritesh Dinkar Pawar**, Radisav Vidic

Paper 381aa: Comparison of Methods of Incorporating Silver into Ultrafiltration Membranes to Prevent Biofouling

— Cannon Hackett, Audie Thompson, David M. Ford

Paper 381ab: Investigation of the Sulfur Adsorption Capability of Ion-Exchange Y Zeolites Using Density Functional Theory and IR Spectroscopy

— **Kevin X. Lee**, Stavros Caratzoulas, George Tsilomelekis, Julia A. Valla

Paper 381ac: Synthesis of Amine-Functionalized Zeolite for Carbon Dioxide Separation

— **Geetanjali Bhati**, Ramgopal V. S. Uppaluri**, Bishnupada Mandal**

Paper 381ad: Direct Air Capture of CO₂ Using Zeolites for the Production of High Purity CO₂

— **Sean Wilson**, F. Handan Tezel

Paper 381ae: Hydrogen Sulfide Removal from Carbon Dioxide-Containing Gas Mixture on "Molecular Basket" Sorbents

- Wenying Quan

Paper 381af: CO₂ Separation Process Based on Temperature Swing Adsorption Using Fluidized Bed — Yasuki Kansha, Masanori Ishizuka

Paper 381ag: Enhanced CO₂ Adsorption Rate in Polyammonium Protic Ionic Liquids Functionalized SBA-15

— Wei Zhang, Yao Shi, Yi He

Paper 381ah: Enhanced Transport Characteristics for the Electrochemically Driven Highly Selective Separation of Gases

— **Philip Cox**, Vincent Storhaug, Kayla O'Neill, Brinkley Artman

Paper 381aj: Effect of Organic Matters on the Fractional Crystallization Process of High-Saline Wastewater from Coal Chemical Industry

— **Chao Bian**, Hang Chen, Xingfu Song, Jianguo Yu

Paper 381ak: Thermal Cross-Linking and Cyclodehydration Modifications of PI Membranes for Pervaporation Applications

— Sheng Xu, Yan Wang

Paper 381al: Application of High-Shear Wet Milling to an API Crystallization Process

— **Joshua R. Dunetz**, Jonathan V. Trinidad, Timothy Chang, Ernest Carra, Bing Shi, Chiajen Lai, Kenneth S. Matthews

Paper 381am: Study on Impurity Control of 7-Adca Isomers

— **Ying Li**, Baoshu Liu, Junli Zhang, Hua Sun, Bowen Du

Paper 381an: Study on Recrystallization of Cephalosporanic Acid G

— **Kang Han**, Baoshu Liu, Junli Zhang, Hua Sun Paper 381ao: Study on the Crystallization Process of Tazobactam Intermediate

- HuiMei Li, Hua Sun, Baoshu Liu

Paper 381ap: Study on the Crystallization Process of 7-Adca Pivaloamide

- Weikai Han, Baoshu Liu, Hua Sun

Paper 381aq: Separation and Crystallization of Solid-Liquid Mixtures — *Qiong Liu*, *Baoshu Liu*, *Hua Sun*

Paper 381ar: Purification of Ethylene with Anion-Pillared Metal-Organic Frameworks As Adsorbents

— **Qi Ding**, Xili Cui, Zhaoqiang Zhang, Lifeng Yang, Huabin Xing

Paper 381as: Oligo-Ethylene-Glycol Based Thin-Film Composite Nanofiltration Membranes for Effective Separation of Mono-/Di-Valent Anions — Dan Ren

Paper 381at: Fabrication of DD₃R Zeolite Membranes on Hollow Fibers for Highly-Selective Separation of CO₂/CH₄

and H₂/CH₄ Mixtures
— *Yuting Zhang*, *Xuehong Gu*

Paper 381au: Tailoring Molecular Architecture of Heterogeneous Nanostructure for High CO₂ Separation Performance

— **Jae Eun Shin**, Ho Bum Park

Paper 381aw: Innovative Graphene Based Membranes for Gas Separation with Tunable Selective Properties

— Giacomo Foli, Simone Ligi, Ferruccio Doghieri, Vincenzo Palermo, **Matteo Minelli**

Paper 381ax: Polybenzimidazole-Derived Carbon Molecular Sieves with Microcavities and Ultra-Microporous Channels Achieving Superior Membrane H./CO., Separation Properties

— **Hien Nguyen**, Maryam Omidvar, Liang Huang, Haiqing Lin, Cara M. Doherty, Anita J. Hill

Paper 381ay: Pure and Mixed Gas Transport and Physical Aging in Glassy Polymers Exhibiting Configurational Free Volume

— Yafei Li, Valerio Loianno, Ryan D. Crist, Shuangjiang Luo, Qinnan Zhang, Ruilan Guo, **Michele Galizia**

Paper 381az: A Thin Film Composite Membrane Prepared from Monomers of Guaiacol and Trimesoyl Chloride for Organic Solvent Nanofiltration

— Ayang Zhou

Paper 381ba: Crystallization Solvent Design Methodology for Pharmaceutical Processes Based on Crystal Morphology Quantitative Control

— Shiyang Chai, Linlin Liu, **Qingwei Meng**

Paper 381bb: Computer-Aided Design of Crystallization Solvents for the Recovery of High-Purity 2-Mercapotobenzothiazole

Mercapotobenzothiazole
— Shiyang Chai, Qilei Liu, Xinyuan
Liang, Yansuo Guo, Song Zhang,
Chengqiu Xu, Lei Zhang, **Jian Du**,
Zhihong Yuan, Rafiqul Gani

Paper 381bc: Enriching Trace
Bioactive Compound and Isolation of
Pesticides from Natural Materials Using
Scalable Supercritical CO₂ Continuous
Countercurrent Extraction

— **Yaping Zhao**, Mulugeta Guta, Minghua Sun

(382) Poster Session: Thermodynamics and Transport Properties (Area 1A)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Andrew Paluch, Chair

Sponsored by: Thermodynamics and Transport Properties

MACROMOLECULES, POLYMERS, AND BIOMOLECULAR SYSTEMS

Paper 382a: Modelling of Ultrasonic Polymer Degradation Using Continuous Kinetics

— Sabine Enders**, David Kruppa**

Paper 382d: Application of Plasticized PEMA/PMMA Sensing Film for Sorption of BTEX Compounds in Vapor Phase Using a Quartz Crystal Microbalance (QCM) at 298.15 K

— **Deekshitha Adapa, Abhijeet Iyer**, Scott W. Campbell, Venkat R. Bhethanabotla

Paper 382e: Pre-Transition Effects and Self-Assembly of Proteins in Multi-Component Lipid Membranes

— Clay H. Batton, Shachi Katira, Kranthi K. Mandadapu

■ MODELING OF PHASE BEHAVIOR

Paper 382f: A Cubic Equation of State for Compounds with No Critical State — Angelo Lucia, Arthur S. Gow

Paper 382g: One-Dimensional Models As Reference States for Predicting Properties of Quasi-1D Inclusion Complexes

— **J. Matthew Mansell**, Erik E. Santiso, Keith E Gubbins

Paper 382h: Thermodynamic Modeling of CaSO₄-(NH₄)₂SO₄-NH₃-H₂O Quaternary System with Asymmetric E-NRTL Model

— **Teng Pan**, Youwei Cheng, Lijun Wang, Xi Li

Paper 382i: Modeling of Excess Molar Volumes for Binary Liquid Mixtures Containing Water and Amines

— Gustavo V. Olivieri, **Ricardo B. Torres**

Paper 382j: Calculation of Hansen Solubility Parameters Based on Solvatochromic Dye

— **Tamura Takuya**, Hideki Yamamoto Sr.

Paper 382k: An Approximate Density-Based Phase Envelope Construction Method

— Dan Vladimir Nichita

Paper 382I: Inferring Broken Detailed Balance in the Absence of Observable Currents

— Gili Bisker

Paper 382m: Phase Equilibrium

Modeling for Biodiesel Reaction Systems

— Allan Albuquerque, Flora Ng,
Leandro Danielski, Luiz Stragevitch

Paper 382n: Improving the Subset Selection Regression of Helmholtz Energy Equations

- Marissa Engle, Nikolaos V. Sahinidis

Paper 382o: Vapor–Liquid Equilibria of Mixtures of Thiophene and n-Hexane Using Monte Carlo Simulations

— Tamaghna Chakraborti, **Jhumpa Adhikari**

Paper 382p: Prediction of Vapor-Liquid Coexistence for Carvacrol Using Equation of State Methods and Monte Carlo Simulations

— **Suryadip Bhattacharjee**, Jhumpa Adhikari

Paper 382q: The Role of Mathematical Artifacts in Deteriorating the Physical Behavior in SAFT Theories

— **Nayef Alsaifi**, Mohammed Alkhater, Housam Binous, Isa Al Aslani, Yousef Alsunni, Zhen-Gang Wang

Paper 382r: Improve Understanding of the Temperature-Dependence of Liquid Viscosity of Organic Compounds through Quantitative Structure-Property Relationship and Correlation

— **Jeremy W. Passey**, Thomas A. Knotts IV, Neil Giles, W. Vincent Wilding

Paper 382s: Predicting and Understanding Azeotrope Formation and Solubility Enhancement Using Mosced

— Julia Ullmann, Rachel Ollier, **Andrew Paluch**

Paper 382t: Predicting Phase Behavior and Intuitive Solvent Selection Using Mosced

— Andrew Paluch

■ MEASUREMENT OF PROPERTIES

Paper 382u: Density, Speed of Sound and Viscosity for Binary Liquid Mixtures Containing Gamma-Valerolactone (GVL) + Ethanol at Different Temperatures — Robert L. Fernandes, Ricardo B.

— кореп L. Fernanaes**, кіс Torres**

Paper 382v: Viscometric Properties of Binary Mixtures of Dimethyl Carbonate with Alcohols at *T* = (288.15 - 308.15)

— Tamires P. Mercês, Ana Beatriz S. Lopes, **Heloisa E. Hoga**, Ricardo B. Torres

Paper 382w: Evaluation of Thermal Conductivity for Binary Liquid Systems Using Binary Vapor-Liquid Equilibrium Data

— **Katsumi Tochigi**, Hiroyuki Matsuda, Kiyofumi Kurihara, Toshitaka Funazukuri

Paper 382x: Molecular Calculation of the Critical Parameters of Classical Helium

— Richard A. Messerly, Navneeth Gokul, Andrew J. Schultz, David A. Kofke, **Allan H. Harvey** Paper 382y: Anthracene-Phenanthrene-Solvent and Phenanthrene-Carbazole-Solvent Ternary Phase Diagrams and Their Applications in the Separation of Them — Suping Ding, Qiuxiang Yin, Hongxun

Paper 382z: Study on Separation and Transformation of Cefuroxime Axeomer — Zhefan Zhang, Baoshu Liu, Junli Zhang, Hua Sun

IONIC LIQUIDS

Paper 382aa: Viscometric Properties of Binary Liquid Mixtures Containing (Acetonitrile + C₄-C₅ Alcohols) at Different Temperatures and Atmospheric Pressure

— João V.M. Castro, Heloisa E. Hoga, Ricardo B. Torres

Paper 382ab: Analysis of Interactions between Ionic Liquid Cations and Enzymatic Core of Cytochrome P-450 in a Quantum Mechanical (QM) Framework — Atiya Banerjee, Jindal K. Shah

Paper 382ac: Structural and Transport Properties of the Mixtures of Ionic Liquid 1-Ethyl-3-Methylimidazolium Dicyanamide and Trifluoroethanol from Molecular Simulations

— **Pratik Dhakal**, Jindal K. Shah

Paper 382ad: High-Pressure
Densities and Derived Properties for
Binary Mixtures Containing 1-Ethyl3-Methylimidazolium-Thiocyanate +
Alcohols

— Daniel B. Hauk, **Ricardo B. Torres**, José Vicente H. D'Angelo

Paper 382ae: Excess Properties of Binary Mixtures of Ionic Liquid Sec-butylammonium Methanoate with 1-Pentanol at *T* = (293.15 – 313.15) K — Heloisa E. Hoga, Robert L. Fernandes, Ricardo B. Torres

Paper 382af: Volumetric Properties of Sucrose in Aqueous 1-Butyl-3-Methylimidazolium Hydrogen Sulfate Ionic Liquid Solution at Different Temperatures

— Rafael N. Pietro, Heloisa E. Hoga, Ricardo B. Torres

Paper 382ag: Prediction of the CO₂ Solubility in Ionic Liquids: A Comparison between Cubic and Group Contribution Equations of State

— Olamide Animasahun, Muhammad Khan, Sheraz Bashir, **Cornelis Peters**

■ PROCESSES

Paper 382ah: Modeling of Wet Flue Gas Desulfurization Process for Merchantable Gypsum Production Using Low Grade Limestone

— **Jonghun Lim**, Yeongryeol Choi, Geonyeol Kim, Dong-hyun Kim, Junghwan Kim

Paper 382ai: Novel and Scalable Approach to Biphilic Patterned Surface for Water Condensation Heat Transfer

— Jiayu Song, King Lun Yeung

Paper 382aj: CFD Study for Optimal Operating Condition in Multi-Stage Packing Scrubber

— **Geonyeol Kim**, Il Moon, Man sig Lee, Dong-hyun Kim, Junghwan Kim

(383) Poster Session: Upstream Engineering and Flow Assurance Tuesday, Nov 12, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

Mohammad Tavakkoli, Chair Francisco Vargas, Co-Chair Vikram Subramani, Co-Chair Kiran Gawas, Co-Chair Andrey Filippov, Co-Chair Michael P. Hoepfner, Co-Chair

Sponsored by: Upstream Engineering and Flow Assurance Forum

Paper 383a: Modelling Ice and Wax Deposition in a Pipeline in the Arctic Environment

— **Hongfei Xu**, Ben Bbosa, Michael Volk, Zhengdong Cheng, Sam M. Mannan

Paper 383b: Towards Field Wide Production Optimization for Upstream Field Recovery; A Holistic Analysis and Optimisation Framework of the Upstream Field from Reservoir to Host Facility.

- Shakeel Ramjanee

Paper 383c: Settling Characteristics of Weighting Material in the OIL-Based Drilling Fluids

— **Dinesh V. Kalaga**, Manizheh Ansari, Sanjoy Banerjee, Masahiro Kawaji, Richard Gyland, Bjorner Lund

Paper 383d: Use of Eco-Friendly Amine Based Hydrate Inhibitors for Hydrate Mitigation and Offshore Flow Assurance — Majeda Khraisheh, M. Fahed

Paper 383e: Investigating the SI Hydrate Crystal Formation at Different Produced Water Levels for Offshore Flow Assurance

— Majeda Khraisheh, M. Fahed Qureshi

(384) 3D Printing of Composites Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 28 Holly A. Stretz, Chair Jason E. Bara, Co-Chair

Sponsored by: 3D Printing

3:30 Keynote

Qureshi

3:40 Paper 384a: Reprocessable 3D-Printed Conductive Elastomeric Composite Foams for Strain and Gas Sensing

— **Peiran Wei**, Houming Leng, Qiyi Chen, Rigoberto Advincula, Emily Pentzer

4:00 Paper 384b: Computational Printing of Cement-Based Pastes with Time-Dependent Rheology

— **Abdul Salam Mohammad**, Joseph J. Biernacki **4:20** Paper 384c: Selective
Nanoparticle Orientation for Polymer
Composites Via Hybrid Manufacturing
— Sayli Jambhulkar, Weiheng Xu,
Kenan Song

4:40 Paper **384d:** Two-Color Photoinitiation / Photoinhibition for Continuous Stereolithographic Additive Manufacturing

— **Martin de Bee**r, Zachary D. Pritchard, Timothy F. Scott, Mark A. Rurns

5:00 Paper **384e**: Direct Ink Writing of Modified Cellulose Nanocrystals

— *Roneisha Haney*, *Subramanian*

(385) Advanced Nuclear Energy Applications for Molten Salts Tuesday, Nov 12, 3:30 PM

Ramakrishan

Hyatt Regency Orlando, Discovery 43
Michael F. Simpson, Chair
Raluca Scarlat, Co-Chair

Sponsored by: Nuclear Engineering Division

- **3:30** Paper 385a: Design and Operation of a System for the Preparation of a Molten Chloride Nuclear Fuel Salt
- **Justin McAllister**, Michael F. Simpson
- **3:50** Paper 385b: Neutron Radiography for the Determination of Molten Chloride Viscosity, Density, and Homogeneity
- **Matt Jackson**, Marisa Monreal, Scott Parker, Alexander Long, Sven Vogel, Bjorn Winkler
- **4:10 Paper 385c:** Electrochemical Corrosion Measurements in Molten Flinak Salt
- **Suhee Choi**, Andrew Strianese, Michael F. Simpson
- **4:30** Paper 385d: Thermodynamic Analysis of Minor Components in Molten Salt Mixtures
- **Richard L. Fitzhugh**, John Harb, Matthew Memmott
- **4:50 Paper 385e:** Metal Dissolution in Molten Salts for Redox Control
- **Olivia Dale**, Suhee Choi, Michael F. Simpson
- **5:10 Paper 385f:** Electrochemical Study on the Corrosion of Structural Materials
- **Haiyan Zhao**, Eugene Engmann, Meng Shi
- **5:30** Paper 385g: Development of Neutron Measurements for in-Situ Interface Corrosion Kinetics and Salt Properties
- **Li (Emily) Liu**, Kemal Ramic, Jinghua Feng

(386) AIChE Journal Futures: New Directions in Chemical Engineering Research (Invited Talks)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Rainbow Spring I/II

Michael Harold, Chair Prodromos Daoutidis, Co-Chair

Sponsored by: Publication Committee

3:30 Paper 386a: Colloidal Self-Assembly of Mechanically-Reinforced Organohydrogels

— Lilian Hsiao

3:55 Paper **386b**: Translocation of Cell-Penetrating Peptides into Fungal Cells — *Amy J. Karlsson*

4:20 Paper 386c: Organic Solvent Reverse Osmosis Separations of Hydrocarbons Using "Polymer-Derived" Membranes

- Ryan Lively

4:45 Paper 386d: Global Optimization of Stiff Dynamical Systems

- Matthew D. Stuber

5:10 Paper **386e**: Impact of Surface Loading on Catalytic Activity of Regular and Low Micropore SBA-15 in the Knoevenagel Condensation

— **Nicholas Brunelli**, Nitish Deshpande, Eun Hyun Cho, Ashwin Kane, Li-Chiang Lin

5:35 Paper 386f: Machine Learning Predictions of Electronic Couplings for Charge Transport Calculations of P₃HT — *Eric Jankowski*

(387) Area 8D (Inorganic Materials) Graduate Student Award Session Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 16 Kumar Varoon Agrawal, Chair Xueyi Zhang, Co-Chair

Sponsored by: Inorganic Materials

Wei Fan, Co-Chair

- **3:30 Paper 387a:** Ultrathin Graphene Oxide-Based Membrane for Separation of Small Organic Molecules
- **Bratin Sengupta**, Qiaobei Dong, Fanglei Zhou, Dinesh Behera, Huazheng Li, Georges Belfort, Miao Yu
- **3:48** Paper **387b**: Reversible On/Off Modulation of Photoluminescence from TiO₂/CsPbBr₃ Using Redox Clusters
- **Azzah Dyah Pramata**, Yuji Akaishi, Armando T. Quitain, Tetsuya Kida
- **4:06** Paper **387c**: A Theoretical Model Based on a Group Contribution Method to Describe Atomic Layer Deposition of Zirconia on Silicon
- **Nickolas D Anderson**, Soumya Saha, Rajib Mukherjee, Christos G. Takoudis, Urmila M. Diwekar
- **4:24** Paper **387d:** Reduced Wrinkling in GO Membrane By Grafting Basal-Plane Groups for Improved Gas and Liquid Separations
- **Han Lin**, Shailesh Dangwal, Ruochen Liu, Seok-Jhin Kim, Yifan Li, Jiahua Zhu

4:42 Paper 387e: Distinct Catalytic Reactivity of Sn Substituted in Framework Locations and at Defect Grain Boundaries in Sn-Zeolites — *Jason S. Bates, Brandon C. Bukowski, James W. Harris, Jeffrey Greeley, Rajamani Gounder*

5:00 Paper 387f: Atomically Dispersed Metal Sites in Multifunctional Zeolite Catalyst for Cascade Ethanol Conversion to C₃-C₆ Olefins

— **Junyan Zhang**, Shiba Adhikari, Ce Yang, Evan C. Wegener, Jeff Miller, Theodore Krause, Junyan Zhang, Lawrence Allard, Dongxia Liu, Zhenglong Li

5:18 Paper 387g: Tailoring the Bioactivity of Flame-Made Nanoparticles for Surgical Applications By Modifying Synthesis Conditions

— Martin T. Matter, Fabian Starsich, Andrea Schlegel, Sotiris E. Pratsinis, Inge K. Herrmann

5:36 Paper **387h**: Single-Layer Graphene Membranes with a Record Performance in Hydrogen Purification and Carbon Capture

— **Shiqi Huang**, Jing Zhao, Kumar Varoon Agrawal

(388) Area 8E (Electronic and Photonic Materials) Graduate Student Award Session (Sponsored by JVST)

Tuesday, Nov 12, 3:30 PM
Hyatt Regency Orlando, Celebration 15
Letian Dou, Chair
Charles Hages, Co-Chair

Sponsored by: Electronics and Photonics

- **3:30 Paper 388a:** Improving Stability and Thin-Film Fabrication Efficiency of Lead-Halide Perovskites
- Atefe Hadi, Matthew G. Panthani
- **3:55 Paper 388b:** Engineering of Ruddlesden-Popper Planar Faults in Cesium Lead Halide Perovskite Nanocrystals
- **Maria Morrell**, Xiaoqing He, Guangfu Luo, Arashdeep Thind, Tommi White, Jordan Hachtel, Albina Borisevich, Juan-Carlos Idrobo, Rohan Mishra, Yangchuan Xing
- **4:20** Paper 388c: Catalyst-Free and Morphology-Controlled Growth of 2D Perovskite Nanowires for Polarized Light Detection
- **Debjit Ghoshal**, Tianmeng Wang, Hsin-Zon Tsai, Michael Crommie, Nikhil Koratkar, Sufei Shi
- **4:45** Paper 388d: Reversible Tuning of the Optoelectronic Properties of Transition Metal Doped Semiconductor Materials for Adaptive Luminescence
- **Pragathi Darapaneni**, Orhan Kizilkaya, James A. Dorman
- **5:10** Paper **388e:** Synthesis and Ligand Engineering of Impurity Free Cu(In,Ga) S₂ Nanoparticles for Slot-Die Coated Photovoltaics
- **Ryan Ellis**, Rakesh Agrawal

- **5:35** Paper 388f: Extreme Temperature Operation of Ultra-Wide Bandgap AlGaN Polarization-Doped Field Effect Transistors
- **Patrick Carey IV**, Fan Ren, Andrew Armstrong, Brianna Klein, Andrew Allerman, Erica Douglas, Albert Baca, Stephen J Pearton

(389) Artificial Intelligence and Advanced Computation

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 27 Helen Durand, Chair Joseph Scott, Co-Chair

Sponsored by: Next-Gen Manufacturing

- **3:30** Paper 389a: A Review and Outlook on Machine Learning and Data Science in Chemical Engineering *Joe Qin, Yining Dong*
- **3:47** Paper **389b**: Neural Network-Based Modeling and Operation for ALD of SiO_2 Thin Films Using Data from a Multiscale CFD Simulation
- **Yangyao Ding, Yichi Zhang**, Zhe Wu, Panagiotis D. Christofides
- **4:04** Paper **389c:** Keynote Talk: Intelligent Cloud-Based Algorithms for Pharmaceutical Drug Development
- **Michael A. Bellucci**, Mingjun Yang, Guangxu Sun, Virginia Burger, Xuekun Shi, Yang Liu, Peiyu Zhang, Jian Ma, Alan Jiang, Shuhao Wen
- **4:31** Paper 389d: Industrial Success Stories with Machine Learning and Deep Learning in Matlab
- **Aycan Hacioglu**, Samvith Rao
- **4:48** Paper 389e: Keynote Talk: Modern Data Analytics to Accelerate the Design of Advanced Materials *Dongwon Shin*
- **5:15 Paper 389f:** GPU-Accelerated Computation of Stirred Tanks *Shuli Shu*, *Ning Yang*
- **5:32** Paper 389g: Keynote Talk: Faster Prediction with Artificial Intelligence: Using Process Simulations and Production Data to Develop Fast-Running Inference Models for Manufacturing
- Victor Castillo

(390) Biomass Thermal Deconstruction via Fast Pyrolysis Biorefineries

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom U Mark Mba Wright, Chair Robert C. Brown, Co-Chair

Sponsored by: Sustainable Biorefineries

- **3:30 Paper 390a:** Understanding the Role of Partial Oxidation Reactions during Autothermal Pyrolysis
- Chad Peterson, Jake K. Lindstrom, Joseph Polin, Preston A. Gable, Robert C. Brown

- **3:55 Paper 390b:** Structural and Chemical Changes in Plant Cell Walls during Early Stages of Thermal Deconstruction
- Jake K. Lindstrom, Chad Peterson, Peter N. Ciesielski, John Ralph, Mingjie Chen, Joseph Jakes, Preston A. Gable, Robert C. Brown
- **4:20 Paper 390c:** Multiscale Simulation of Autothermal Pyrolysis of Biomass
- Peter N. Ciesielski, Brennan Pecha, Hariswaran Sitaraman, Gavin Wiggins, Charles E. A. Finney, Jim Parks, Xi Gao, Deepthi Chandramouli, Bill Rogers
- **4:45** Paper 390d: Significant Increase in the Production of Sugars from Pyrolysis of Agricultural Residues By Application of Iron Sulfate Pretreatment
- **Sean A. Rollag**, Joseph Polin, Preston A. Gable, Andrew Friend, Jake K. Lindstrom, Robert C. Brown
- **5:10** Paper **390e**: A Novel Fluidized Bed Model for Fast Pyrolysis Applications
- **Benjamin Caudle**, Maxmilian Gorensek, Chau-Chyun Chen
- **5:35 Paper 390f:** CFD Investigation of Autothermal Biomass Pyrolizers
- **Barlev Nagawkar**, Venkata S. P. Kotrike, Shankar Subramaniam, Alberto Passalacqua

(391) Biomaterials for Immunological Applications

Tuesday, Nov 12, 3:30 PM
Hyatt Regency Orlando, Celebration 3
Catherine A. Fromen, Chair
John Wilson, Co-Chair
Kyung-Ho Roh, Co-Chair
Carolina Salvador-Morales, Co-Chair

Sponsored by: Biomaterials

- **3:30 Paper 391a:** Targeting Translocator Protein 18kDa (TSPO) Improves Mitochondrial and Tumor-Specific Targeting of PAMAM Dendrimers in Glioblastoma
- **Kevin Liaw**, Anjali Sharma, Sujatha Kannan, Rangaramanujam Kannan
- **3:48** Paper 391b: Cytokine-independent, Physiologic Production of Dendritic Cells via Platelet P-selectin for Immunotherapy
- Patrick Han, Doug Hanlon, Najla Arshad, Kazuki Tatsuno, Eve Robinson, Renata Filler, Jungseok Lee, Christine Cote, Felix Rivera-Molina, Tarek Fahmy, Richard Edelson
- **4:06 Paper 391c:** Encapsulating Proteins into Complex Coacervates
- **Sarah L. Perry**, Whitney C. Blocher McTigue, Abigail Cabral, Shari Traiger
- **4:24** Paper **391d:** Polyanhydride Nanoparticles Activate Dendritic Cells and Enhance CD₈+ T Cell Memory Response Leading to Delayed Tumor Progression
- Ross Darling, Sujata Senapati, John
 Christiansen, Luman Liu, Michael J.
 Wannemuehler, Balaji Narasimhan

- **4:42** Paper **391e**: Oxime Crosslinked Alginate Hydrogels with Tunable Stress Relaxation for Immune CELL Encapsulation
- Hector Sanchez-Moran, **Kyung-Ho Roh**
- **5:00** Paper 391f: Magnetic Particle Imaging for Quantitative Tracking of Adoptive Cell Transfer in Cancer Immunotherapy
- Angelie Rivera-Rodriguez, Lan Hoang-Minh, Leyda Marrero-Morales, Duane A. Mitchell, Carlos Rinaldi
- **5:18** Paper **391g**: Multimodal Multiplexed Immunoimaging with Gold Nanostars
- **Rizia Bardhan**, Yu-Chuan Ou, Xiaona Wen
- 5:36 Paper 391h: Dual Functional Immunostimulatory Polymeric Prodrug Carrier with Pendent Indoximod for Enhanced Cancer Immunochemotherapy
- Zhuoya Wan

(392) Biomaterials: Graduate Student Award Session

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 2 Ryan Koppes, Chair Kaitlin M. Bratlie, Co-Chair Shreyas Rao, Co-Chair Iman Noshadi, Co-Chair

Sponsored by: Biomaterials

- **3:30 Paper 392a:** Graduate Student Award Session: Galactosylated Dendrimer Targets Hepatocytes and Improves Therapeutic Outcomes in a Severe Model of Acetaminophen Poisoning
- **Joshua E. Porterfield**, Rishi Sharma, Anjali Sharma, Ambar Jimenez, Sam Norwood, Sujatha Kannan, Rangaramanujam Kannan
- **3:44** Paper 392b: Graduate Student Award Session: Stimuli-Responsive Hydrogel Microparticle Populations As a 'Plug and Play' Model for Controlled and Tailorable Therapeutic Delivery

 Paige LeValley, April M. Kloxin
- **3:58 Paper 392c:** Graduate Student Award Session: A Data Analytics Approach for Rational Design of Nanomedicines with Programmable Drug Release
- Adam Mullis, Scott Broderick, Andrea M. Binnebose, Nathan Peroutka-Bigus, Bryan H. Bellaire, Krishna Rajan, Balaji Narasimhan
- **4:12** Paper **392d:** Graduate Student Award Session: Nanoparticle Hitchhiked T Cells for Targeted Drug Delivery — *Muhammad Raisul Abedin*, *Yongjian Liu, Sutapa Barua*
- **4:26** Paper **392e**: Graduate Student Award Session: Targeting Translocator Protein 18kDa (TSPO) Improves Mitochondrial and Tumor-Specific Targeting of PAMAM Dendrimers in Glioblastoma
- **Kevin Liaw**, Anjali Sharma, Sujatha Kannan, Rangaramanujam Kannan

- **4:40** Paper 392f: Graduate Student Award Session Design of a Slow-Releasing Antioxidant Drug Delivery System for Stroke
- Nicholas Murphy, Kyle Lampe
- **4:54** Paper **392g**: "Graduate Student Award Session:"Investigating the Concurrent Effect of Encapsulation and Perfusion on Chondrogenic Differentiation of Mesenchymal Stem Cells
- **Amin Vossoughi Shahvari**, Howard W. T. Matthew
- **5:08** Paper **392h**: Bio-lonic Liquid Conjugated Hydrogels As Hemostatic Adhesives
- **Vaishali Krishnadoss**, Tyler Hannah, Ethan Ellis, Andy Kapetanakis, Iman Noshadi
- **5:22 Paper 392i:** Graduate Student Award Session: Physical Intimacy of Glioblastoma Cells with Astrocytes Elicits Metabolic Reprogramming of Glioma Cells
- **Kimberly M Stanke**, Christina Wilson, Oleh Khalimonchuk, Srivatsan Kidambi
- 5:36 Paper 392j: Graduate Student Award Session: 3D-Bioprinting of Spatially Organized Bacterial Microcosmoi Using Chaotic Flows — Carlos Fernando Ceballos-González, Carolina Chávez-Madero, Everardo González-González, Juan Felipe Yee-de León, Christian Carlos Mendoza-Buenrostro, Y. Shrike Zhang, Mario Moisés Álvarez, Grissel Trujillo-de Santiago

(393) Bionanotechnology Graduate Student Award Session II

Tuesday, Nov 12, 3:30 PM
Hyatt Regency Orlando, Discovery 45
Lorraine Leon, Chair
Catherine A. Fromen, Co-Chair
Elizabeth Nance, Co-Chair

Sponsored by: Bionanotechnology

- **3:30** Paper **393a**: Award Submission: Quantum Capacitance Based Amplified Graphene Phononics for Studying Neurodegenerative Diseases
- Bijentimala Keisham, Akop Seksenyan, Steven Denyer, Pouyan Kheirkhah, Gregory Arnone, Pablo Avalos, Abhiraj D. Bhimani, Clive Svendsen, Vikas Berry, Ankit Mehta
- **3:50** Paper **393b:** Lipid Membrane Bilayer Destabilization By Amphiphilic Coumarin: A Biophysical Study for Cancer Applications
- **Poornima Kalyanram**, Anju Gupta, Istvan Stadler
- **4:10** Paper 393c: Award Submission: Engineering Muco-Inert Nanoparticles for Improved Vaginal Drug Delivery during Pregnancy
- Hannah Zierden, Jairo I. Ortiz, Kevin DeLong, Peter Dimitrion, Victoria Laney, Sabrine Bensouda, Justin Hanes, Laura Ensian

- **4:30** Paper **393d**: Award Submission: Xeno Nucleic Acid Nanosensors for Enhanced Stability *Alice J. Gillen, Justyna Kupis-Rozmysłowicz, Carlo Gigli, Nils Schuergers, Ardemis A. Boghossian*
- **4:50 Paper 393e:** Award Submission: Development of a Model Placental Lipid Bilayer
- **Christina Bailey-Hytholt**, Tun-Li Shen, Anubhav Tripathi, Anita Shukla
- 5:10 Paper 393f: Award Submission:Sequence and Aggregation State Determine Stability, Endosomal Processing, and Long-Term Fate of DNA-Wrapped Carbon Nanotubes in Mammalian Cells
- **Mitchell Gravely**, Mohammad Moein Safaee, Daniel Roxbury
- **5:30** Paper **393g**: Award Submission: Real-Time Detection of H₂O₂ Signaling in Wild-Type Plants with Nanobionics Approach
- Tedrick Thomas Salim Lew, Volodymyr Koman, Seonyeong Kwak, Kevin Silmore, Michael Strano

(394) Chemical Engineering Principles Advancing Medicine

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 12/13

Christopher L. Burcham, Chair Thomas A. Zangle, Co-Chair

Sponsored by: Chemical Engineers in Medicine

- 3:30 Welcoming Remarks
- **3:33** Paper **394a**: Customized Medicine for in-Vitro Fertilization (IVF) Using Modeling and Optimal Control Apporva Nisal, Urmila M. Diwekar
- **3:54** Paper **394b**: Computational Fluid Dynamics Simulations of the Human Carotid Artery to Predict Strokes in Patients with Carotid Artery Disease *David G. Foster*, *Anna Weldy*, *Amanda Forti*
- **4:15** Paper **394c:** Personalized Treatment of Sickle Cell Disease Using Hydroxyurea Pharmacokinetic-Pharmacodynamic Modeling
- **Akancha Pandey**, Robert Hannemann, Peter Kissinger, Seethal Jacob, Terry Vik, Sangtae Kim, Doraiswami Ramkrishna
- **4:36** Paper **394d:** Antioxidant-Encapsulating Nanoparticles for the Treatment of Glutamate Excitotoxicity — *Rick Liao, Elizabeth Nance*
- **4:57** Paper **394e:** Engineering Variable Lymphocyte Receptors to Target Blood Brain Barrier Disruption Via Exposed Neural ECM
- **Benjamin J. Umlauf**, Paul A. Clark, Brantley R. Herrin, John S. Kuo, Eric V. Shusta
- **5:18** Paper **394f**: Effect of Screening Compliance on Optimal CRC Screening Policies
- **David Young**, Selen Cremaschi

- **5:39** Paper 394g: An Approach Towards Method Development for Untargeted Urinary and Serum Metabolite Profiling in Metabolomics Research, As a Tool in Exposome Studies, Using Uplc-Q-TOF/MS
- **Dimosthenis Sarigiannis**, Nafsika Papaioannou, Aikaterini Gabriel, Spyros Karakitsios

(395) Climate Solutions

Tuesday, Nov 12, 3:30 PM

Hyatt Regency Orlando, Silver Spring

Hyatt Regency Orlando, Silver Spring I/II **Tom Rehm, Chair**

Sponsored by: Climate Solutions

- 3:30 Welcoming Remarks
- **3:45 Paper 395a:** AIChE Climate Change Policy Review Process – New Policy
- Mary Ellen Ternes
- **4:15 Paper 395b:** Plastics and Greenhouse Gas Emissions
- Jeffrey R. Seay
- **4:45** Paper **395c:** Getting to Zero: Options for Decarbonizing Electricity in the United States
- Jesse Jenkins
- **5:15 Paper 395d:** Climate Solutions' Path Forward
- Tom Rehm
- 5:45 Concluding Remarks

(396) Concentrated Solar Energy for Power Generation and Chemical Processing III

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom T

Alexandre Yokochi, Chair Nick AuYeung, Co-Chair Wojciech Lipinski, Co-Chair Christopher L. Muhich, Co-Chair

Sponsored by: Concentrated Solar Energy for Power Generation and Chemical Processing

- **3:30 Paper 396a:** Performance Characteristics of a Directly-Irradiated Windowless Solar Vortex Particle Receiver
- **Alfonso Chinnici**, Dominic Davis, Woei L. Saw, Zhao Tian, Graham J. Nathan
- **3:55** Paper **396b:** Non-Thermal Equilibrium Heat Transfer Model of a Thermochemical Solar Reactor Based on Porous Media
- Aldo J. Guadarrama-Mendoza, Carlos E. Arreola-Ramos, Heidi I. Villafán-Vidales, Camilo A. Arancibia-Bulnes, Patricio J. Valadés-Pelayo, Juan D. Macias
- **4:20 Paper 396c:** Attenuation of Absorber End Loss in Parabolic Trough Collectors
- Mohammad Abutayeh
- **4:45** Paper 396e: Modal Switching for Continuous Solar Reforming of Methane *Lucas Freiberg, Fuqiong Lei, Nick AuYeung*

- **5:10 Paper 396f:** Sustainable Steam on Demand for the Bayer Process
- Andrew Beath, Alicia Bayon

(397) Conversion of Solid Wastes to Energy and/or Product

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Regency Ballroom Q Zheng Liu, Chair Hsi-Wu Wong, Co-Chair

Michael Tai, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

- **3:30** Paper 397a: Chempren: A New Technology for the Conversion of Mixed Municipal Waste to Basic Chemicals and Fuels
- Anne Gaffney, Gennaro J. Maffia, Amanda Peterman, Xufung Liu, Lynn M. Wendt
- **3:45** Paper **397b:** Anaerobic Digestion of Food Wastes into Energy and Fertilizer
- **Yen Wah Tong**, Jingxin Zhang, Kai Chee Loh
- **4:00 Paper 397c:** Subcritical Water Upgrading of Coal Refuse with Food Waste
- Shanta Mazumder, Pretom Saha, **M.Toufiq Reza**
- **4:15** Paper **397d**: Synthesis and Characterization of Hydrochars Produced By Hydrothermal Carbonization of Banana Peels
- **Ifrah Yusuf**, Bogdan Dorneanu, Claudio Avignone-Rossa, Harvey Arellano-Garcia
- **4:30 Paper 397e:** Polar Solvents Facilitate Efficient Microwave Pretreatment of Woody Biomass
- Akshat Tanksale**, Negin Amini**, Victoria Haritos
- **4:45** Paper 397f: Comparative Leading Pretreatments for Improving Lignin Waste Valorization to Biobased Products *Zhi-Hua Liu*, *Joshua Yuan*
- **5:00** Paper **397g**: Waste to Resource: Synthesis of Electrolyte and Electrode Material in Vanadium Redox Flow Battery from Leachate of Industrial Waste
- He Li, Chi-Hwa Wang
- **5:15 Paper 397h:** Synthesis of LiNi_{0.6} Co_{0.2}Mn_{0.2}O₂ Cathode Material By a Carbonate Co-Precipitation from Spent Lithium-lon Batteries
- **Lei Xing**, Shuying Sun, Sen Lin, Ping Li, Jianguo Yu
- **5:30 Paper 397i:** Sustainable Process for the Recycling of Polyethylene Phthalate
- Zheng Liu
- **5:45 Paper 397j:** Recycling Fe-P Slag As Energy Materials Via a Green Technics
- **Guixin Wang**, Yun Wei, Fei Xu, Jiangdong Zou, Shunxing Wang

(398) Developments in Shale Gas, LNG, CNG, and LPG

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Challenger

Karthikeyan K. Ramasamy, Chair Umakanta Jena, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

- **3:30** Paper 398a: Full-Scale Simulation, Energy and Environmental Analysis of an Actual LNG Chain *Mary Katebah*, *Mohamad Hussein*, *Abdur Rahman Shazed*, *Zineb Bouabidi*,
- Abdulla Al-Hajri, Easa Al-Musleh **3:51 Paper 398b:** Replacing Steam with Methane in Thermal Cracking
- Processes

 Wasiu P. Oladipupo, Abhijit
 Talpade, Jeffrey J. Siirola, Fabio H.
- Ribeiro, Rakesh Agrawal

 4:12 Paper 398c: Comparative
 Study on Helium Recovery and
 Purification from LNG Liquefication
- **Tarun K Gupta**, Yogesh Kurle, Qiang Xu. Sriniyas Palanki
- **4:33** Paper 398d: Determination of the Failure Envelope of Kerogen Matrix By Molecular Dynamics Simulations
 Tianhao Wu. Abbas Firoozabadi
- **4:54** Paper 398e: Modeling of Methane Recovery from Gas Hydrate Particle Decomposition Under Fluidized Conditions
- Airong Li, Dan Luo

Process

- **5:15 Paper 398f:** CFD Based Dynamic Boil-Off Gas Study during LNG Laden Voyage
- Xingchun Wang, Qiang Xu
- **5:36** Paper **398**g: Static Boil-Off Rate (BOR) Implication on Boil-Off Gas (BOG) in an LNG Regasification Terminal *Mohd Shariq Khan*
- (399) Division Plenary: Food, Pharmaceutical, and Bioengineering

Division (Invited Talks)
Tuesday, Nov 12, 3:30 PM
Hyatt Regency Orlando, Regency
Ballroom V

Shelly Peyton, Chair Joshua N. Leonard, Co-Chair William Bentley, Co-Chair

Sponsored by: Food, Pharmaceutical & Bioengineering Division

- **3:30** Paper 399a: Reflections on Enabling a Better Biomanufacturing Ecosystem: Ambic and Beyond...

 Michael Betenbaugh
- **4:30** Paper 399b: Novel Bioelectrochemical Bioreactor Systems for Enhanced Biosynthesis Processes *An-Ping Zeng*
- **5:00 Paper 399c:** Microdroplet-Enabled Metabolic Engineering and Directed Evolution
- Hal Alper

5:30 Paper 399d: Reprogramming Stem Cell Rejuvenation for Tissue Regeneration

- Stelios T. Andreadis

(400) Emulsions and Foams Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom J Amir M. Farnoud, Chair Esteban Urena-Benavides, Co-Chair

Claribel Acevedo, Co-Chair

Sponsored by: Interfacial Phenomena

- **3:30 Paper 400a:** Three Dimensional Multiphasic Structures Via Vaporization Induced Phase Separation (VIPS)
- **Tiancheng Wang**, Giuseppe Di Vitantonio, Daeyeon Lee, Kathleen J. Stebe
- **3:45** Paper **400b**: Advective Flow in Bicontinuous Interfacially Jammed Emulsion Gels (bijels) for Continuously Operated Liquid-Liquid Extraction
- **Stephen Boakye-Ansah**, Mohd Azeem Khan, Martin F. Haase
- **4:00** Paper **400c**: Foaming
 Performance of Anti-Foam Laden
 Lubricants Subject to Filtration
 Vineeth Chandran Suja, Abhishek
 Kar, Gerald G. Fuller
- **4:15** Paper **400d**: Geometry, Surfactant and Droplet Crystal Content Control Partial Coalescence
- **Samira Abedi**, Chau-Chyun Chen, Siva A. Vanapalli
- **4:30 Paper 400e:** Interfacial and Molecular Interactions between Cellulose Nanocrystals and Surfactants in Brine and Responsible for Pickering Emulsion Stability
- **Sanjiv Parajuli**, Leeta Prater, Kevin Green, Trey Heath, Esteban E. Ureña-Benavides
- **4:45 Paper 400f:** Predicting Emulsions Stability Using Coarse-Grained Simulations
- Abeer Khedr, Alberto Striolo
- **5:00** Paper **400**g: Kinetic Analysis of Oil Exchange between Emulsion Droplets Using Small Angle Neutron Scattering
- Yi-Ting Lee, Lilo Pozzo
- **5:15** Paper 400h: Structures of Surfactant Systems at the Oil/Water Interface Zengyi Wei, Andrew Nelson, Patrick T. Spicer, Stuart W. Prescott
- **5:30** Paper **400i**: Effect of Spacer Nature on Foaming Properties of Cationic Gemini Surfactant
 Shams Kalam, Shirish Patil, **Muhammad Shahzad Kamal**, SM Shakil Hussain

(401) Entrepreneurship in Chemical Engineering: Transitioning from the Lab to the Boardroom

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom N Amy Beaird, Chair

Sponsored by: Entrepreneurship in Chemical Engineering - Sponsored by CIEE

- **3:30 Paper 401a:** Presentation by Frana James, CEO, Allied Microbiota *Frana James*
- **4:00** Paper **401b:** Presentation by Hannah Murnen, CTO, Compact Membrane
- Hannah Murnen
- **4:30 Paper 401c:** Presentation by Roger Pettman, Executive Chairman, Cycladex Inc
- Roger Pettman
- **5:00 Paper 401d:** Presentation by Santiago Rojas-Carbonell, COO, W,energy LLC
- Santiago Rojas-Carbonell
- **5:30 Paper 401e:** Presentation by George Diloyan, CEO, Nanotech Industrial Solutions
- George Diloyan

(402) Excellence in Graduate Polymer Research (Invited Talks)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 5 Samanvaya Srivastava, Chair Jessica D. Schiffman, Co-Chair

Sponsored by: Polymers

- **3:30** Paper 402a: Scalable and Facile Preparation of Self-Healable Single-Ion-Conducting Networks (SSN) for Lithium Metal Stabilization
- **David Mackanic**, Zhiao Yu, Yi Cui, Zhenan Bao
- **3:45 Paper 402b:** Crosslinkable Nitroxide Radical Polymer for Energy Storage Applications
- **Shaoyang Wang**, Alexandra Easley, Fei Li, Jodie L. Lutkenhaus
- **4:00 Paper 402c:** Investigating the Effect of Salt on Segmental Dynamics in Block Copolymer Electrolytes for Lithium Batteries
- **Whitney S. Loo**, Antonio Faraone, Nitash P. Balsara
- **4:15** Paper 402d: Tuning Charge and Energy Transfer Interactions in Open-Shell Molecules
- **Daniel A. Wilcox**, Bryan W. Boudouris
- **4:30 Paper 402e:** Impact of Nanoparticle Aggregation on Ion Transport and Nanostructure in Ionomer Nanocomposite Membranes
- **Allison Domhoff**, Apoorv Balwani, Tyler Martin, Ronald L. Jones, Eric M. Davis

- **4:45** Paper **402f**: Local Density and Free Volume Inhomogeneities Govern Transport Properties in Reverse Osmosis Membranes
- **Tyler E. Culp**, Manish Kumar, Enrique D. Gomez
- 5:00 Paper 402g: 2D-Macromolecular Heterostructures Enabled Memristive Colloidal Particle
- Albert Tianxiang Liu, Pingwei Liu, Daichi Kozawa, Juyao Dong, Jing Fan Yang, Volodymyr Koman, Max Saccone, Michael Strano
- **5:15 Paper 402h:** Electrospinning Coacervates No Chain Entanglements Required
- Xiangxi Z. Meng, Yifeng Du, Yalin Liu, E. Bryan Coughlin, Sarah L. Perry, Jessica D. Schiffman
- **5:30** Paper **402i**: Long-Lived Self-Entanglements in Ring Polymers

 — *Beatrice W. Soh*, Alexander Klotz, Patrick S. Doyle
- **5:45** Paper **402**j: Design of Polymeric Cryoprotectants for Quantitative Post-Thaw Recovery of Mammalian Cells after Storage at –196 °C
- Aaron A. Burkey, Nathaniel A. Lynd

(403) Experiences in Teaching Process Safety II

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 17 Z. Otero Gephardt, Chair Nastassja Lewinski, Co-Chair Benjamin J. Davis, Co-Chair

Sponsored by: Product Design

- **3:30 Paper 403a:** A Perspective on Teaching Process Safety through the Curriculum
- Kenneth R. Cox
- **3:55 Paper 403b:** An Initiative on Safety across the Chemical Engineering Curriculum Scott Fogler
- H. Scott Fogler
- **4:20** Paper 403c: Learning Hazards of Exothermic Reactions Via Real and Virtual Experiments
- William M. Clark
- **4:45 Paper 403d:** Fundamental Approaches to Reactive Chemicals Hazard Recognition and Analysis
- Jessica E. Nichols, Robert J. Bellair
- **5:10 Paper 403e:** New Liquid Flammability Rating with the Assist of Machine Learning
- **Shuai Yuan**, Joseph Sang-II Kwon, Chad Mashuga

(404) Fuel Cells, Electrolyzers, and Electrochemical Devices

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 29/30 Ryan Anderson, Chair Burcu Gurkan, Co-Chair

Sponsored by: Transport and Energy Processes

- **3:30** Paper **404a**: In-Situ Electrochemical Techniques to Determine Ionomer Coverage in PEFC Electrodes
- **Timothy Van Cleve**, Sunilkumar Khandavalli, Samantha Medina, Svitlana Pylypenko, Scott A. Mauger, K.C. Neverlin
- **3:45 Paper 404b:** Overpotential Analysis of Low Loading Pt/C Electrodes Developed By Reactive Spray Deposition Technology
- **Ryan Ouimet**, Haoran Yu, Leonard Bonville, Radenka Maric
- **4:00 Paper 404c:** Rechargeable Aluminum-Graphite Batteries: Elucidation of Ionic Transport and Intercalation Reaction Limitations Via Electrochemical Analyses
- **Jeffrey Xu**, Damon Turney, Ankur Jadhav, Robert J. Messinger
- **4:15 Paper 404d:** Modeling the Transport of Nitrogen in Gas Diffusion Electrode (GDE) for the Electrochemical Ammonia Synthesis at Ambient Conditions
- **Nishithan C. Kani**, Aditya Prajapati, Meenesh R. Singh
- **4:30** Paper **404e:** Hexachloroiridate As an Alternative to Hexacyanoferrate in Electrochemical Mass Transfer Measurements
- **Stéphane Weusten**, Mattheus de Groot, John van der Schaaf
- **4:45** Paper **404f**: Ptir/IrOx on Fluffy TiO₂ /CNTs As a Catalyst for Methanol Oxidation
- Ahmed Jasim, Yangchuan Xing
- **5:00** Paper **404g:** Critique of Maximum Power Point Tracking in Open-Cathode Direct Methanol Fuel Cells
- Zuhair Alyousef, Oscar Crisalle
- **5:15** Paper 404h: Investigation of the Microstructure and Rheology of Iridium Oxide Catalyst Inks for Low-Temperature Proton Exchange Membrane Water Electrolyzers
- **Sunilkumar Khandavalli**, Jae Hyung Park, Nancy N. Kariuki, Deborah J. Myers, Michael Ulsh, Scott A. Mauger
- **5:30 Paper 404i:** Demystifying Mass Transfer in Electrolyzers through 3D Printed Parallel Plate Cells: The Importance of Inlet Effects
- **Stéphane Weusten**, Luc Murrer, Mattheus de Groot. John van der Schaaf
- **5:45** Paper **404j**: Ni-Based Cermet Anode with a Three-Dimensionally Ordered Macroporous Structure for Solid Oxide Fuel Cells
- Yongdan Li

(405) Fundamentals and Applications for Municipal Solid Waste Treatment and Valorization

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Blue Spring I/II Robert W. Peters, Chair Eunsung Kan, Co-Chair Matthew L. Alexander, Co-Chair

Sponsored by: Solid and Hazardous Waste

- 3:30 Paper 405a: Overview of Waste Valorization Concepts and Principles -Robert W. Peters, Jeffrey R. Seay
- 3:51 Paper 405b: Conversion of Polyvinylchloride Containing Solid Wastes into Value-Added Products — Joel Braden**, Xianglan Bai**
- 4:12 Paper 405c: Development of High Performance Composites Using Recycled Materials
- -Haibin Ning, Robert W. Peters, Siddhartha Brahma, Selvum Pillay
- 4:33 Paper 405d: Sustainable Mass-Burn Refuse-Derived-Fuel-to-Energy System: A Municipal Solid Waste Management Case Study -Tapas Das, Robert W. Peters
- 4:54 Paper 405e: Investigation of Reactions at the Gas/Solid Interface of Municipal Solid Waste Residues Tasnuva Moutushi, Marco J.

Castaldi

- 5:15 Paper 405f: Microwave Enhanced Advanced Oxidation Treatment of Anaerobic Digested Effluent
- Moutoshi Saha, Asha Srinivasan, Ping Huang Liao, Kwang Victor Lo

(406) Fundamentals of **Computational and Experimental** Catalysis

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom F Neeraj Rai, Chair Praveen Bollini, Co-Chair

Sponsored by: Catalysis and Reaction **Engineering Division**

- 3:30 Paper 406a: Operando Surface Enhanced Raman Spectroscopy Study of the Oxygen Reduction Reaction on a Non-Model Pt Catalyst
- **Sean T. Dix**, Suljo Linic
- 3:48 Paper 406b: Comparative Analysis of HxWO, Bronze Formation through Thermochemical and **Electrochemical Routes**
- Evan V. Miu, Giannis Mpourmpakis, James R. McKone
- 4:06 Paper 560ck: pH Effects in the Hydrogen Oxidation Reaction: A DFT/MD Approach to Understand Adsorbed Hydroxyl on Platinum
- Jon Wilson, Stavros Caratzoulas, Dionisios G. Vlachos, Yushan Yan
- 4:24 Paper 406d: Probing Hydroxyl Groups on Metal-Supported 2-D Silica Films
- Angela M. Norton, Weiqing Zheng, Dionisios G. Vlachos, Michael Tsapatsis, Jorge A. Boscoboinik
- 4:42 Paper 406e: Ab Initio Population Balance Model of TiCl, Grafting on Amorphous Silica
- Salman Khan. Baron Peters. Susannah L. Scott

- 5:00 Paper 406f: Acceleration of Methanol Dehydration in H-SSZ-13 By Acid Site Proximity
- Alexander Hoffman, John R. Di Iorio, Steven V. Nystrom Jr., Claire T. Nimlos, Rajamani Gounder, David
- 5:18 Paper 406q: Oxidant-Free Dehydrogenation of 2,3-Butanediol to 3-Hydroxy Butanone on Metal Catalysts: A Combined Experimental and Computational Study
- Kelvin Mingyao Kwok, Jithin John Varghese, Tanachaporn Panyathanakun, Daniel Sze Wei Ong, Samir H. Mushrif, Luwei Chen, Armando Rorana
- 5:36 Paper 406h: Automated Microscopic Reaction Path Analysis of Methane Dehydrogenation on Ptsn Catalysts
- Tibor Szilvási, Duygu Gerceker, Benjamin Wei Jie Chen, Manos Mavrikakis

(407) Graphene 2-D Materials: Synthesis, Functions and **Applications II**

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Discovery 44 Lei Li, Chair Sanjay Behura, Co-Chair

Sponsored by: Carbon Nanomaterials

- 3:30 Paper 407a: Atomically-Precise Moiré Fringes in 2D Van Der Waals Heterostructures of Graphene and Hexagonal Boron Nitride
- Sanjay Behura, Songwei Che, Phong Nguyen, Chen Wang, Rousan Debbarma, Michael R. Seacrist, Vikas Berry
- 3:50 Paper 407b: UV Surface Plasmon Resonance Modification By Graphene Pi Plasmon Resonance
- Xueling Cheng, Sourangsu Banerji, Jieying Mao, Sara Arezoomandan, Ting Zhang, Steve Blair, Berardi Sensale-Rodriguez, Yunshan Wang
- 4:10 Paper 407c: Temperature **Dependent Photovoltaic Characteristics** of Graphene/h-BN/Si Solar Cell
- Chen Wang, Sanjay Behura, Vikas Berry
- 4:30 Paper 407d: Graphene-Based Passivation of Liquid Metal Particle
- Megan A. Creighton, Zachary Farrell, Benji Maruyama, Christopher
- **4:50 Paper 407e:** 3D-Printed Graphene/Polymer Structures for **Electron-Tunneling Based Devices**
- Deisy Cristina Carvalho Fernandes, Dylan Lynch, Vikas Berry
- 5:10 Paper 407f: Cross-Linked Reduced Graphene Oxide Aerogels and Their Applications As 3D Electrodes for Lithium-Ion Batteries
- Han Xiao, Joshua Pender, C. Buddie Mullins, Christopher J. Ellison

(408) Hydrodynamics of Biological **Systems**

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom L

Pushkar Lele, Co-Chair Amy M. Peterson, Co-Chair

Sponsored by: Fluid Mechanics

- 3:30 Paper 408a: Influence of Rheological Models in a Pulsatile Flow inside a Generic Carotid Artery Aneurysm with the Use of Computational Hemodynamics - Cristian R. Schwatz, Igor A. D. Fiamoncini, Marcela K. Silva, Ricardo N. Sousa, Leonardo M. Rosa, Henry F.
- 3:45 Paper 408b: In Vivo Measurement of Blood Clot Strength from Computational Fluid Dynamics Based on Intravital Microscopy Images

Meier, Jaci C. S. C. Bastos

- Roman Voronov, Olufemi Kadri, Migle Surblyte, Vishnu Deep Chandran, Danh Nguyen, Cortes Williams III, Vassilios I. Sikavitsas
- 4:00 Paper 408c: Blood Group Alters Platelet Binding Kinetics and Translocation Dynamics Under Arterial
- Qin M. Qi, Eimear Dunne, Ingmar Schoen, Antonio J. Ricco, James O'Donnell, Dermot Kenny, Eric S. G. Shaqfeh
- 4:15 Paper 408d: Cross-Stream Distribution and Dynamics of Red Blood Cells in Sickle Cell Disease
- Xiao Zhang, Wilbur A Lam, Michael D. Graham
- 4:30 Paper 408e: Interspecies Variations in Hemorheology and Hemodynamics
- **Jeffrey S. Horner**, Yu-Jiun Lin, Antony N. Beris, Norman J. Wagner
- 4:45 Paper 408f: Determining How Human Mesenchymal Stem Cells Change Their Degradation Strategy in Response to Microenvironmental Stiffness
- Maryam Daviran, Jenna Catalano, Kelly M. Schultz
- 5:00 Paper 408g: Swimming Bacteia at Complex Fluid Interfaces
- Mehdi Molaei, Jiayi Deng, Nicholas G. Chisholm, Kathleen Stebe
- 5:15 Paper 408h: Hydrodynamic Trapping of Bacteria Near Walls - **Debasish Das**, Eric Lauga
- 5:30 Paper 408i: Microbially-Induced Emulsification of Hexadecane By Marinobacter sp₁₇
- George E. Kapellos. Nicolas Kalogerakis, Patrick S. Doyle
- 5:45 Paper 408j: Investigating the Influence of Polysorbate 20/80 and Polaxomer P₁₈₈ on Bovine Serum Albumin and Lysozyme Aggregation, Rheology & Interfacial Properties — Farzana Begum**, Samiul Amin**

(409) In Honor of Yannis Kevrekidis' 60th Birthday (Invited Talks)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Florida Ballroom B

T. J. Mountziaris, Chair Stanislav Y. Shvartsman, Co-Chair

Sponsored by: Catalysis and Reaction **Engineering Division**

- 3:30 Paper 409a: Learning in Control — Manfred Morari
- 3:49 Paper 409b: Accelerating and Enhancing Chemical Synthesis By Integrating Machine Learning, Automation, and Robotics - Klavs F. Jensen
- 4:08 Paper 409c: Computational Studies of DNA Hybridization — Pablo G. Debenedetti
- 4:27 Paper 409d: Modeling What We Don't Know: Disturbance Models and Model Predictive Control
- James B. Rawlings
- 4:46 Paper 409e: Cross Flow Reactor Design for Fischer-Tropsch Synthesis: Analysis of Dynamic Behavior - Moshe Sheintuch
- 5:05 Paper 409f: Pattern Formation on Surfaces of Strained Thin Films
- Dimitrios Maroudas 5:24 Paper 409g: Embryogenesis: A
- Cascade of Dynamical Systems - Stanislav Y. Shvartsman
- 5:43 Paper 409h: Deep Learning of Low-Dimensional Latent Space Molecular Simulators
- Hythem Sidky, Andrew Ferguson

(410) Innovations and Emerging **Technologies: Drug Substance and Drug Product Development**

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 8 Tim Boung-Wook Lee, Chair Mohammad Azad, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 410a: Formulating Biologics in Polymeric Nanoparticles: New Methods to Overcome Manufacturing Barriers — Chester E. Markwalter, Robert F

Pagels, Robert K. Prud'homme

- 3:51 Paper 410b: Co-Immobilization of Enzyme Cascades Enables One-Pot Industrial Immobilized Biocatalysis - Jacob H. Forstater, Rachel S. Bade, Sandra A. Robaire, Chihui An, Joshua N. Kolev, Shane T. Grosser
- 4:12 Paper 410c: Application of Membrane Technology for Metal Removal from a Reaction Mixture - Manish S. Kelkar, Mike Rasmussen, John Hartung, Harsit Patel, Thaddeus Franczyk, Onkar Manjrekar, Geran

Zhang, Elie Chaaya, Nandkishor K. Nere

- **4:33 Paper 410d:** Applications of Soft Sensors in Pharmaceutical Manufacturing Processes
- **Zilong Wang**, Reza Kamyar, Hamidreza Mehdizadeh
- **4:54 Paper 410e:** Process Performance of a Novel Continuous Process Line for Drying of an Active Pharmaceutical Ingredient
- Isabella Aigner, Manuel Zettl, Markus Krumme, Thomas Mannschott, Peter van der Wel, Johannes G. Khinast
- **5:15** Paper **410f**: On-Demand Drug Product Manufacturing in a Miniaturized System: Can Formulation be Simplified?
- **Mohammad Azad**, Juan G. Osorio, Allison Wang, David Klee, Mary Eccles, Erin Grela, Rebecca Sloan, Gregory Hammersmith, Kersten Rapp, David Brancazio, Allan Myerson
- **5:36** Paper **410g**: Slow Freezing Process Design for Human Induced Pluripotent Stem Cells By Modeling Intracontainer Variation
- Yusuke Hayashi, Ikki Horiguchi, Masahiro Kino-oka, **Hirokazu Sugiyama**

(411) Innovations in Methods of Data Science

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Peacock

Andrew White, Chair Srinivas Rangarajan, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

- **3:30 Paper 411a:** Big Data from Sparse Data: Diverse Scientific Benchmarks Reveal Optimization Imperatives for Implicit Membrane Energy Functions
- **Rebecca F. Alford**, Patrick Fleming, Jeffrey J. Gray
- **3:45** Paper **411b**: Actively Learning Robust High-Complexity Force Fields *Rebecca Lindsey*, *Laurence E. Fried*, *Nir Goldman*, *Sorin Bastea*
- **4:00 Paper 411c:** Data Analytics for Designing Fe-9Cr Steels (Tensile Strength)
- **Vyacheslav N. Romanov**, Jeffrey A. Hawk
- **4:15** Paper **411d:** Transfer Learning with Autoencoder Latent Spaces: A Novel Framework for Improved Chemical Prediction from Scarce Datasets
- Brett Savoie
- **4:30 Paper 411e:** Advancing Machine Learning Methodology for the Chemical and Materials Domain
- Johannes Hachmann
- **4:45 Paper 411f:** HOOMD-TF: Online Machine Learning in Molecular Dynamics Simulations
- **Rainier Barrett**, Maghesree Chakraborty, Dilnoza Amirkulova, Heta Gandhi, Andrew White

- **5:00 Paper 411g:** Study of Density Functional Errors in Microkinetic Modeling: A Data Driven Approach
- **Himaghna Bhattacharjee**, Dionisios G. Vlachos
- **5:15** Paper **411h:** Using Molecular Subgraph Libraries for High-Throughput Screening and the Inverse Design Problem
- Nick Austin
- **5:30 Paper 411i:** Convolutional Network Analysis of Optical Micrographs for Liquid Crystal-Based Sensors
- **Alexander Smith**, Nicholas L. Abbott, Victor M. Zavala
- **5:45 Paper 411j:** Uncertainty Measurement Method for Machine Learned Potentials
- Ni Zhan, John R. Kitchin

(412) LGBTQ+ Inclusion in Engineering

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 23 Stephanie Farrell, Co-Chair Gayle Gibson, Co-Chair Anthony Butterfield, Co-Chair

Sponsored by: Engineering for Inclusion

(413) Lignin for Sustainable Industrial Uses

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Discovery 47 Amar K. Mohanty, Chair Manju Misra, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

- **3:30** Paper 413a: Codesign of Combinatorial Organosolv Pretreatment (COP) and Lignin Nanoparticles (LNPs) in Biorefineries
- **Zhi-Hua Liu**, Arthur J. Ragauskas, Joshua Yuan
- **3:50 Paper 413b:** Tailoring the Molecular Weight of Purified Lignins for Materials Applications
- **Junhuan Ding**, Graham W. Tindall, Carter Fitzgerald, Mark C. Thies
- **4:10** Paper **413c**: Multi-Stream Integrated Bioproducts Enabled By Biorefinery Lignin Waste Fractionation
- **Qiang Li**, Cheng Hu, Mengjie Li, Joshua Yuan
- **4:30 Paper 413d:** Light-weight Carbonaneous Biocomposites for Auto-parts uses
- Amar K. Mohanty
- **4:50 Paper 413e:** Upgrading Lignin Side-Streams into Sustainable Ligniox Plasticizers and Dispersants
- **Anna Kalliola**, Tapio Vehmas, Tiina Liitiä, Petteri Kangas, Mathilde Fiorletta, Erasmo Cadena
- **5:10** Paper **413f**: Synthesis of Acrylated Thermoplastic Polymers from Crude Lignin Bio-Oil: Effect of Intrinsic Properties of Crude Bio-Oil and Synthesis Conditions
- **Yixin Luo**, Wangda Qu, Eric W. Cochran, Xianglan Bai

5:30 Paper 413g: The Role of Different Hydroxyl Groups in Promoting Coke Formation during Lignin Pyrolysis

— Yuan Xue

(414) Mathematical Modeling of Transport Processes

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom I Norman W. Loney, Chair

Sponsored by: Transport Processes

- **3:30 Paper 414a:** Acoustothermal Heating in a Surface Acoustic Wave Driven Microchannel
- **Pradipta Das**, Arthur David Snider, Venkat R. Bhethanabotla
- **3:43** Paper **414b**: Analysis of the Biodegradation of Dilute Oil-in-Water Emulsions Using a Compound Particle-in-Cell Model
- **George E. Kapellos**, Nicolas Kalogerakis, Patrick S. Doyle
- **3:56** Paper **414c**: Drying Kinetics of Single Droplet of Sugar Cane Molasses *Valeria D. Benalcazar, Paulo Cesar Narváez Rincón, Alvaro Orjuela*
- **4:09** Paper **414d:** Kinetic Model for Polyelectrolyte Migration Induced By a Combination of Shear and Electric Fields *Jason E. Butler*, *Dmitry I.*
- Jason E. Butler, **Dmitry Kopelevich**
- **4:22 Paper 414e:** Solution of the Full Bgk Model of the Boltzmann Transport Equation Using Alternating Least Squares
- **Arnout Boelens**, Daniele Venturi, Daniel Tartakovsky
- **4:35** Paper **414f**: Nonequilibrium Thermodynamics of Diffusion and Chemical Reactions in Multicomponent Systems
- **Antony N. Beris**, Soham Jariwala, Norman J. Wagner
- **4:48 Paper 414g:** Interpenetrating Mixture Theory
- Charles A. Petty, André Bénard
- **5:01** Paper **414h:** A Flexible Model Fidelity for Simulating Vapor Sorption and Diffusion in Porous Media
- **Yunwei Sun**, Hom Sharma, Pratanu Roy, Stephen Castonguay, Jennifer M. Knipe, Sarah Matt, Elizabeth Glascoe
- **5:14 Paper 414i:** A Comprehensive Analysis of Transient Heat Conduction in Solid Slabs Using Tailor-Made Integral Transforms
- Satish J. Parulekar
- **5:27** Paper **414j**: Transient Finite Element Modeling of Coupled Diffusion and Triple-Mode Sorption in Porous Polymers
- **Stephen Castonguay**, Pratanu Roy, Hom Sharma, Elizabeth Glascoe, Yunwei Sun
- **5:40 Paper 414k:** Direct Numerical Simulation of Mass Transfer of a Rising Deformable Bubble
- **Chengxiang Li**, Xiaogang Shi, Yingya Wu, Jinsen Gao, Xingying Lan

- **5:53** Paper **414**!: A Liquid Maxwell-Stefan Diffusion Coefficient Prediction Model Derived from Entropy Generation Minimization Principle
- **Shengkun Jia**, Xuepu Cao, Xing Qian, Xigang Yuan

(415) Mechanics, Structure, and Properties in Polymers

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 14 Xue (Ida) Chen, Chair Mingjiang Zhong, Co-Chair

Sponsored by: Polymers

- **3:30 Paper 415a:** Local Chain Alignment Via Nematic Ordering Reduces Chain Entanglement in Conjugated Polymers
- Enrique D. Gomez
- **4:00** Paper **415b**: Molecular Architecture Effects on Polymer Viscoelasticity: An Expansion of the Van Gurp Palmen Methodology
- Zhiyuan Qian**, Gregory B. McKenna**
- **4:15 Paper 415c:** Synthesis and Processing of High-Strength and High-Toughness Crystalline 2-D Covalent Organic Frameworks
- Morgan Barnes, Dongyang Zhu, Qiyi Fang, Jia Liang, Muhammad Rahman, Ashok Kumar, P.M. Ajayan, Jun Lou, Rafael Verduzco
- **4:30 Paper 415d:** Examining the Impact of Dispersity on Functional Polymers
- Jimmy Lawrence
- **4:45** Paper **415e:** The Effect of As-Spun Fiber Morphology on Post Drawn Ultra High Molecular Weight Polyethylene Fiber Performance
- Christopher Henry, Giuseppe Palmese, **Nicolas J. Alvarez**
- **5:00** Paper **415f**: Polymer Chain Sequence Effects on the Glass Transition *William F. Drayer*, *David S. Simmons*
- **5:15** Paper 415g: Ultra-Stretchable Conductive Polymer Complex with Excellent Linearity and Repeatable Autonomous Self-Healing Ability

 Yang Lu, Evan K. Wujcik
- **5:30 Paper 415h:** Granular Composite-Enabled Tissue-like Dynamic Responsive Materials
- **Yin Fang**, Endao Han, Yuanwen Jiang, Yiliang Lin, Xianghui Xiao, Jin Wang, Heinrich M. Jaeger, Bozhi Tian
- **5:45** Paper 415i: Water-Soluble Fluorescent Perylene Dye Supramolecular Polymers with Controlled Chain Length *Wang Ying*

(416) Microfluidic and Nanoscale Flows: Separations and Particulates

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom M Sujit S. Datta, Co-Chair Amanda B. Marciel, Co-Chair

Sponsored by: Fluid Mechanics

- **3:30** Paper **416a**: Inertial Migration of Neutrally Buoyant Prolate and Oblate Spheroids in Plane Poiseuille Flow Using Dissipative Particle Dynamics Simulations
- Yuanding Huang, Ryan L. Marson, Ronald G. Larson
- **3:45** Paper **416b**: Particle Migration in a Liquid-Liquid Stratified Flow in a Microchannel
- **T. Krishnaveni**, T. Renganathan, S. Pushpavanam
- **4:00** Paper 416c: Cross-Stream Migration of Non-Spherical Particles in a Second Order Fluid Theories of Particle Dynamics in Arbitrary Quadratic Flows (i.e., Pressure Driven Flows) Cheng-Wei Tai Shiyan Wang Vivek
- **Cheng-Wei Tai**, Shiyan Wang, Vivek Narsimhan
- **4:15 Paper 416d:** Lateral Migration of an Electrophoretic Particle in a Viscoelastic Poiseuille Flow
- **A. Choudhary**, T. Renganathan, S. Pushpavanam
- **4:30 Paper 416e:** Holographic Detection of Particles and Cells in the Microfluidic Labyrinth Device
- Anirudh Gangadhar, Siddhartha Gupta, Adity Pore, Swastika S. Bithi, Shamim Ahmmed, Eric Lin, Sunitha Nagrath, Siva A. Vanapalli
- **4:45** Paper **416f**: Electrophoretic Separation of DNA By Normal Stress — *Chih-Hsiang Shu, Chen-Ju Liu, Chun-Shen Chang, Chih-Chen Hsieh*
- **5:00 Paper 416g:** A Model for Solute Macro-Transport in Spatio-Temporally Inhomogeneous Flows: Application to Dispersion in Slip-Stick Channels and Eccentric Annulus
- **Henry C. W. Chu**, Stephen Garoff, Robert D. Tilton, Aditya S. Khair
- **5:15** Break
- **5:30 Paper 416i:** Characterization of Polymeric Nanoparticles Via Microfluidic Interfacial Complexation
- Eric Johnston, Victor M. Ugaz
- **5:45 Paper 416j:** Efficient Transport between Disjoint Nanochannels By Water Bridge
- **Muhammad Sahimi**, Fatemeh Ebrahimi

(417) Nanocomposites with 2D Materials

Tuesday, Nov 12, 3:30 PM
Hyatt Regency Orlando, Celebration 11
Zhengtang Luo, Chair
Amit Nautiyal, Co-Chair

Sponsored by: Composites

- **3:30 Paper 417a:** Edge-Epitaxial Growth of Graphene
- Zhengtang Luo
- **3:55 Paper 417b:** Thermally Conductive Polyethylene-hBN Nanocomposites for Heat Exchanger Applications
- Mehamed Ali, Ahmed Abdala

- **4:20 Paper 417c:** Tunable Hygromorphism: Structural Implications of Molecular Gels and Electrospun Nanofibers in Bilayer Composites
- **Symone Alexander**, LaShanda T.J. Korley
- **4:45** Paper **417d**: Directional Control of Carbonization & Graphitization in Carbon-Carbon Composites By Graphene
- Madhu Singh, Randy Vander Wal
- **5:10** Paper **417e**: Identification of Thermal Barrier Areas in Membranes Assembled with 2D Materials By Using Scanning Thermal Microscopy

 Yifan Li, Han Lin, Jiahua Zhu
- **5:35** Paper **417f**: Permselective H₂/CO₂ Separation and Desalination of Hybrid GO/RgO Membranes with Controlled Pre-Cross-Linking
- **Han Lin**, Ruochen Liu, Shailesh Dangwal, Seok-Jhin Kim, Nitin Mehra, Yifan Li, Jiahua Zhu

(418) Nanomaterials for Hydrogen Production and Fuel Cells I: Fuel Cells

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Discovery 46 Seung Soon Jang, Chair Seung Woo Lee, Co-Chair

Sponsored by: Nanomaterials for Energy Applications

- **3:30 Paper 418a:** Investigation of Highly Nanoporous Metal Oxide Catalysts Via Nano-Template Synthesis for Oxygen Evolution Reaction
- **Chanho Pak**, Seung Woo Lee, Chae Kyung Baik
- **4:00** Paper 418b: Research and Application of Reinforced Composite Polymer Electrolyte Membrane in Fuel Cell for Transportation Applications
- Jin Young Kim
- **4:30** Paper 418c: Strain-Driven Exsolution in Perovskite Oxide for Improved Catalytic Activity at the Anode of Solid Oxide Fuel Cell
- Kyeounghak Kim, Bonjae Koo, WooChul Jung**, Jeong Woo Han**
- **5:00** Paper **418d:** Effect of Side Chain Length in Phosphoric Acid Based Membranes on Nanophase-Segregation and Transport
- **Robin Lawler**, Charles Caliendo Jr., Seung Soon Jang
- **5:20 Paper 418e:** Quantitative Study of the Stability of Colloidal Metallic Nanoparticles with Different Shapes in Reactive Chemical Environments at Atomic Level
- **Xuan Yang**, Marco Dunwell, Yushan Yan, Bingjun Xu
- **5:40** Paper **418f**: Facile One Pot Synthesis of Palladium-Based Alloy Wavy Nanowires for Hydrogen Separation *Abhishek Kumar*, *Liang Huang*, *Haiqing Lin*, *Mark T. Swihart*

(419) Oxygen and Hydrogen Photocatalysis and Electrocatalysis III

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Florida Ballroom A

Ben Meekins, Chair Samira Siahrostami, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30** Paper 419a: Design of Ni-Based Alloys to Improve Electrocatalytic Performance and Sulfur Poisoning Resistance in Solid Oxide Electrochemical Cells
- **Ara Cho**, Jeong Woo Han
- **3:48** Paper **419b:** Atomically Dispersed Ni–Nx Species Anchored Porous Carbon with Embedded Ni Nanoparticles for Efficient Hydrogen Evolution *Yang Hou*
- **4:06 Paper 419c:** Electrochemical Coarsening in Morphologically Complex Electrocatalysts
- Joshua Snyder, Yawei Li
- **4:24 Paper 419d:**Photoelectrochemistry of GaxZn₁-XOyN₁-Y/TiO₂ Heterostructures
- Thomas Ballard, **Ben Meekins**
- **4:42** Paper **419e**: Nitrogen-Coordinated-Iron-Carbon (FeNC) Catalysts for Oxygen Reduction Reaction in Phosphoric Acid Fuel Cells
- Deeksha Jain, **Vance Gustin**, Dishari Basu, Anne Co, Umit S. Ozkan
- **5:00 Paper 419f:** PGM-Free and Iron-Free Catalysts for Oxygen Reduction in PEM Fuel Cells
- Yanghua He, Mengjie Chen**, Gang**
- **5:18** Paper 419g: Compositions, Structures, and Properties of Mesoporous-Fe,N-Containing Carbon Materials for Oxygen Reduction Electrocatalysts
- **Shona Becwar**, Zachariah Berkson, Niels Zussblatt, Donghun Kim, Bradley F. Chmelka
- **5:36 Paper 419h:** Using Operando Characterization Techniques to Uncover the Structure and Composition of Active Sites during Oxygen Reduction Electrocatalysis
- Michaela Burke Stevens,

Melissa Kreider, Brenna Gibbons, Gan Chen, Alessandro Gallo, Zhihua Chen, Shucheng Chen, Zhenan Bao, Apurva Mehta, Ryan Davis, Hirohito Ogasawara, Laurie A King, Thomas F. Jaramillo

(420) Polymer Networks, Gels, and Crosslinked Systems II

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 4 Nese Orbey, Chair Santanu Kundu, Co-Chair

Sponsored by: Polymers

3:30 Paper **420**a: High Temperature Thermoplastic Elastomer Gels

— *Jiaqi Yan*, *Richard J. Spontak*

- **3:45** Paper **420b**: Photorheology and Gelation during Polymerization of Coordinated Ionic Liquids

 Rig D. Corder, Jason F. Barg, Sagu
- **Ria D. Corder**, Jason E. Bara, Saad A. Khan
- **4:00 Paper 420c:** Towards a Mechanistic Understanding of Associative Covalent Adaptable Networks
- Bassil El-Zaatari, Julia Kalow
- **4:15 Paper 420d:** Interrelating Relative Reactivity, Network Topologies, and Thermomechanical Properties in Vinyl-Ester Thermosets Using All-Atom Molecular Simulations
- **Ming Huang**, Cameron F. Abrams
- **4:30** Break
- **4:45** Paper 420e: Recyclable Cross-Linked Polymer Networks Via One-Step Controlled Radical Polymerization
 — Kailong Jin Linguigo Li, John M.
- Kailong Jin, Lingqiao Li, John M.
 Torkelson
- **5:00** Paper 420f: Reprocessable Polymer Networks Based on Dynamic Covalent Bonds: Achievement of Full Crosslink Density Recovery after Recycling and Creep Suppression at High Temperature
- **John M. Torkelson**, Lingqiao Li, Xi Chen, Kailong Jin, Sumeng Hu
- **5:15** Paper **420g:** One-Pot Synthesis of Surface-Anchored Gradient Networks from Common Polymers
- **Pandiyarajan Chinnayan Kannan**, Jan Genzer
- **5:30** Paper **420h**: Beyond Ideal Networks: Understanding Poly(acrylamide)-Based Hydrogel Materials Via Atomistic Modeling *Dylan Anstine, Grit Kupgan, Coray*
- **5:45** Paper **420i**: Photoinitiators Have Predictable Toxicity That Is Protected with N-Acetylcysteine
- **Nicholas Murphy**, Kyle Lampe

M. Colina

(421) Predictive Scale-up/Scale-down for Production of Pharmaceuticals and Biopharmaceuticals I

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 7 Peter Clark, Chair Duygu Gerceker, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **3:30 Paper 421a:** Standing-Wave Design of Three-Zone, Open-Loop Non-Isocratic SMB for Purification
- **David M. Harvey**, Yi Ding, Nien-Hwa Linda Wang
- **3:50 Paper 421b:** Scaling Down to Scale-up: A Multi-Step Recrystallization for Particle Size Control
- **Anthony Moffa**, Naomi Briggs, Jacklyn O'Neil, Daniel Pohlman, Hector Guzman, Mark Tawa, Renato A. Chiarella

- **4:10** Paper **421c**: Solubility-Limited Impurity Purge in Crystallization Theory, Applications and Development Strategies
- Fredrik Nordstrom
- **4:30** Paper **421d:** Understanding the Role of Cake Structure in the Filtration of Needle-like Crystals in the Pharmaceutical Industry
- **Giulio Perini**, William Hicks, Anna R. Parsons, Carlos Avendano, Thomas Vetter
- **4:50 Paper 421e:** The Effect of Particle Sedimentation on the Performance of Pressure Filters
- Ioannis S. Fragkopoulos, **Niall Mitchell**, Claire MacLeod, Suju Mathew,
 Frans L. Muller
- **5:10** Paper **421f**: Removal Dissolved Metal Impurities from API Stream Using Functionalized Silica Resins in a Packed Column
- **Onkar Manjrekar**, Laura McKee, Andrew Ickes, Cynthia Rush, Milad Nazari, John Hartung, Manish Kelkar, Geran Zhang, Elie Chaaya, Jeff Kallemeyn
- **5:30** Paper **421g**: An Approach for Scaling up Jet Milling of Pharmaceutical APIs in Loop Mills of Similar Design *Dolapo Olusanmi, William Bartels*
- **5:45 Paper 421h:** API Micronization Strategy for De-Risking the Pathway to Commercialization
- William Bartels
- (422) Process Research for Improved Throughput & Efficiency, and Reduced Cost

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 18 Rob Nunley, Chair Xue (Ida) Chen, Co-Chair

Sponsored by: Process Research and Innovation

- **3:30** Paper **422a**: Developing a Systematic Approach for the Collaboration between Process Systems Engineering and Catalysis to Accelerate the Improvements of Chemical Processes
- **Abdulrahman S. Alsuhaibani**, Shaik Afzal, Mohamed Sufiyan Challiwala, Nimir O. Elbashir, Mahmoud M. El-Halwagi
- **4:00** Paper **422b**: Novel LNG Boil-Off Gas Re-Liquefaction System Design Using Dual-Mixed-Refrigerant Cycle and an Ejector
- **Jiwon Choi**, Jinwoo Park, Hyungjoon Yoon, Il Moon
- **4:30 Paper 422c:** Crystallization Process Understanding and Optimization Using FBRM and Raman As PAT Tools
- Archana Kumar
- **5:00 Paper 422d:** Design and Synthesis of RNA Thermoregulators to Optimize Production of Essential Metabolites and Therapeutic Molecules in Bioprocesses
- Jose Ruben Morones

- **5:30** Paper **422e**: Techno-Economic Analysis of Emerging Vaccine Platform and Production Technologies: How Can We Produce Vaccines Faster and Cheaper?
- **Zoltán Kis**, Robin Shattock, Cleo Kontoravdi, Nilay Shah

(423) Process-wide and Operational Topics

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 6 Yu Luo, Chair Prashant Kumar, Co-Chair Sudarshan Ganesh, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- 3:30 Break
- **3:51** Paper **423b**: Applications of Real-Time Machine Learning in Process Performance and Product Quality Prediction in Biopharmaceutical Manufacturing
- Michelle (So Young) Park, Seyma Bayrak, Melody Grace Lim, Tom Mistretta
- **4:12 Paper 423c:** A General Framework for Real-Time Risk Assessment in Pharmaceutical Processes: Application to the Automatic Rejection of Off-Spec Oral Drug Doses
- Francesco Rossi, Sudarshan Ganesh, Linas Mockus, Gintaras Reklaitis
- **4:33** Paper **423d**: Towards a Comprehensive Ontology to Describe a Pharmaceutical Product
- **Shekhar Viswanath**, Steve Guntz, Jon Dieringer, Shankar Vaidyaraman, Hua Wana, Chrysanthos E. Gounaris
- **4:54 Paper 423e:** PRIME: Process Ranking of Inputs from Manufacturing and Environment
- Filipe Ataíde, Ana Pimentel, Rui Pina Campos, Miguel Lopes, André S. Ferreira, Rui Pinto, Rui Loureiro
- **5:15 Paper 423f:** Interactive Prior Knowledge Assessments to Predict Process Performance
- **Paul Gramlich**, Kyle McElearney, Nitya Jacob
- **5:36 Paper 423g:** Natural Language Processing What Can Chemistry Learn from Finance?
- **Praful Krishna**, Harshad Kulkarni, Himanshu Gupta, Kalpesh Balar

(424) Reaction Engineering Perspectives for Process Intensification from Industry and Academia (Invited Talks)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom E Amrit Jalan, Chair Kathryn Bjorkman, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30 Paper 424a:** Nature-Inspired Process Intensification
- Marc-Olivier Coppens
- **3:55 Paper 424b:** Process Intensification and Process Scale-up: Gaps and Opportunities
- Bryan Patel, Carla Pereira, Anastasios Skoulidas. James Bielenbera
- **4:20** Paper **424c:** Chemical Reaction Engineering for Process Intensification *Benjamin Wilhite*
- **4:45** Paper **424d:** Use of CRE to Democratize Good Working Practices in the Hydrocarbon Processing Industry of the Future
- Kurt Vanden Bussche
- **5:10 Paper 424e:** Perspectives on Reaction Engineering and Process Intensification
- Jan J. Lerou

(425) Thermochemical CO₂ Reduction II: C2+ Chemicals Tuesday, Nov 12, 3:30 PM

Hyatt Regency Orlando, Plaza International Ballroom D Helena Hagelin-Weaver, Chair Jeremy T. Feaster, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30 Paper 425a:** Selective Hydrogenation of CO₂ over ZSM-5-Based Tandem Catalysts
- Renjie Liu, Marc D. Porosoff
- **3:48** Paper **425b:** Direct Production of Higher α-Olefins from Carbon Dioxide over Iron-Based Catalysts—Catalyst Life Cycle and Reaction Kinetics
- Chenxi Cao, Chao Zhang, Yulong Zhang, Minjie Xu, Xianglin Liu, Jing Xu, Yi-Fan Han
- **4:06** Paper **425c:** Indium Oxide with SAPO-34 Bifunctional Catalyst for CO₂ Hydrogenation to Light Olefins
- **Sunkyu Kim**, Jochen Lauterbach, Erdem Sasmaz
- **4:24** Paper **425d:** Unique Preparation of TiO₂ SWCNT Nanocomposites for the Photocatalytic Conversion of Carbon Dioxide
- Karishma Piler, Tracy J. Benson
- **4:42** Paper **425e**: Highly Efficient Pt-Femo/Ni-Based Al_2O_3 -Ce O_2 Catalysts for Dry-Reforming of Methane
- **Abbas Jawad**, Fateme Rezaei, Ali Rownaghi
- **5:00** Paper **425f**: Ternary Rare-Earth Transition Metal Catalysts for Dry Reforming of Methane, Characterization of Final Structures and Sulfur Tolerance Evaluation
- Changyi Jiang, Michael J. Janik, Bo Li, Emily Loisel, **Kerry M. Dooley**
- **5:18** Paper **425**g: Synergy between Different Active Sites in Affecting CO₂ Hydrogenation Kinetics and Selectivity *Libo Yao, Xiaochen Shen, Yanbo Pan, Zhenmeng Peng*

- **5:36 Paper 425h:** Highly Effective and Economically Viable Catalysts for Gas Phase CO₂ Upgrading
- **Tomás Ramirez-Reina**, Estelle Le Saché, Laura Pastor-Perez

(426) The Role of Solvents in Biomass Upgrading

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Florida Ballroom C

Marc D. Porosoff, Chair Arthur Shih, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30 Paper 426a:** Leaching of Rhenium Species from Oxide-Supported Deoxydehydration Catalysts for Biomass Upgrading: Support, Solvent and Reactant Effects
- Bryan E. Sharkey, Friederike C. Jentoft
- **3:48** Paper **426b**: Effect of Sulfuric Acid and Solvent Environment in the Hydrogenolysis of Glycerol on ReOx-Ir Catalyst: A Combined Experimental and Computational Study
- **Jithin John Varghese**, Liwei Cao, Christopher Robertson, Yanhui Yang, Lynn F. Gladden, Alexei Lapkin, Samir H. Mushrif
- **4:06** Paper **426c:** Understanding the Adsorption and Hydrogenation of Model Bio-Oil Compounds in Aqueous Phase James Akinola, Isaiah Barth, Bryan R. Goldsmith, **Nirala Singh**
- **4:24** Paper **426d:** Effects of Chloride lons in Acid-Catalyzed Biomass Dehydration Reactions in Polar Aprotic Solvents
- Benginur Demir, Max A. Mellmer, Chotitath Sanpitakseree, Kaiwen Ma, William Elliott, Peng Bai, Robert L. Johnson, Theodore Walker, Brent H. Shanks, Robert Rioux, Matthew Neurock, James A. Dumesic
- **4:42** Paper **426e**: The Effect of Solvents and Amine-Functionalized Metal-Organic Frameworks in Glucose Isomerization to Fructose
- **Mohammad Shahinur Rahaman**, Md. Anwar Hossain, Thanh Khoa Phung, Sarttrawut Tulaphol, Mark Crocker, Noppadon Sathitsuksanoh
- **5:00** Paper **426f**: Conversion of Dihydroxyacetone into Lactic Acid over Metal Phosphates Catalysts in a Packed Bed Reactor
- **Giada Innocenti**, Andrew Medford, Giuseppe Fornasari, Fabrizio Cavani, Carsten Sievers
- **5:18** Paper **426g**: Investigation of Thermodynamics and Kinetics of Glycerol Aqueous Phase Reforming Via Multi-Scale Simulations
- Tianjun Xie, Rachel B. Getman
- **5:36 Paper 426h:** Understanding the Colloidal Surface Interactions between Solid Acid Catalysts and Cellulose Using DLVO Theory
- Michael T. Timko, Ziyang Zhang

(427) Topical Plenary: Advances in Fossil Energy R&D (Invited Talks)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Challenger 41/42

Madhava Syamlal, Chair Chunshan Song, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

3:30 Paper 427a: U.S. Department of Energy Fossil Energy R&D Program: Overview and Priorities

— John Wimer

4:00 Paper 427b: Outlook for Energy: A View of 2040

- Vijay Swarup

4:30 Paper **427e**: Driving the Technology Innovation Ecosystem through Applied Research and Collaboration

- Brian Anderson

5:00 Paper **427c**: Energy Conversion and Utilization in Carbon-Constrained World: Carbon Capture, Utilization and Storage (CCUS)

— Ah-Hyung Alissa Park

5:30 Paper 427d: Building Digitally Coupled Learning and Innovation Processes

- Monty Alger

(428) Topical Plenary: Fundamentals of Microbial Interactions with Interfaces (Invited Talks)

Tuesday, Nov 12, 3:30 PM
Hyatt Regency Orlando, Celebration 9
Anita Shukla, Co-Chair
Nancy J. Lin, Co-Chair
Tagbo H.R Niepa, Co-Chair

Sponsored by: Microbes at Biomedical Interfaces

3:30 Paper **428a**: Invited Speaker: The Bacterial Sense of Touch: Chemical and Mechanical Interactions of Bacterial Cells at Interfaces

- Maria M. Santore

3:58 Paper 428b: Invited Speaker: How Bacteria Read the Map: Effects of Surface Topography on Biofilm Formation

- Dacheng Ren

4:26 Paper 428c: Invited Speaker: Motility and Adhesion of Bacteria Near Oil Droplets

— Jacinta C. Conrad

4:54 Paper 428d: Invited Speaker: Transport Phenomena of Microbes in Groundwater and Porous Media

— Roseanne M. Ford

5:22 Paper 428e: Invited Speaker: Goodbye Hospitals: Hello Implantable Nano Sensors

— Thomas J. Webster

5:50 Paper 428f: Concluding Remarks for Microbes at Biomedical Interfaces (Topical Conference)

– Tagbo H.R Niepa

(429) Topical Plenary: Materials Chemistry for Sensor Technology (Invited Talks)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Celebration 10 Jeffrey M. Halpern, Chair

Sponsored by: Sensors

3:30 Introductory Remarks

3:35 Paper **429a**: (Invited Plenary Talk): Reproducibility and Reusability of Surface Bound Electrochemical Sensors

- Jeffrey M. Halpern

4:10 Paper **429b:** (Invited Plenary Talk): Electrochemical Sensors for Multiplexed Infection Detection and Monitoring

- Edgar D. Goluch

4:45 Paper 429c: (Invited Plenary Talk): Hybrid Plasmonic Nanomaterials for Uranium Sensing

— **Amanda Haes**, Hoa Phan

5:20 Paper 429d: (Invited Plenary Talk): Continuous, Real-Time, Physiological Monitoring with Nanosensors

- Kevin J. Cash

5:55 Concluding Remarks

(430) Tribute to Jacob Israelachvili II (Invited Talks)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom K Norma Alcantar, Chair Younjin Min, Co-Chair Kai Kristiansen, Co-Chair

Sponsored by: Interfacial Phenomena

3:30 Paper 430a: Comparison of Line Tension Measurement Methods for Lipid Monolayers at Liquid-Liquid Coexistence — Benjamin Stottrup, Joseph A. Zasadzinski

4:00 Paper **430b**: Equilibrium Forces, Twist Transitions and Metastable States in Cholesteric Liquid Crystal Films Probed with a Surface Force Apparatus

- Bruno Zappone

4:20 Paper 430c: Ion Exchange and DLVO Theory

— Clayton J. Radke, Charles Li, Andrew Crothers

4:40 Paper **430d:** Visualising Reactivity at Electrified Interfaces with the Surface Forces Apparatus: From Corrosion to SEI Formation on Li-Anodes

— Markus Valtiner

5:00 Break

5:20 Paper 430f: Jacob and the Surface Forces Apparatus (SFA)

— Kai Kristiansen

5:40 Paper **430g**: Responsive Coatings from Low-Methoxyl *Opuntia Ficus-indica* Cactus Intended for Controlled Release Applications

— **Zeinab Veisi**, Ryan Toomey, Norma Alcantar

(431) Understanding Mixing Processes II: Experimental and Computational Investigations

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 32 David O. Lignell, Chair Richard Kehn, Co-Chair

Sponsored by: North American Mixing Forum

3:30 Paper 431a: Assessment of 3D-PTV to Measure Lagrangian Flow Fields in Stirred Tanks

— Manuele Romano, Federico Alberini, Mark Simmons, E. Hugh Stitt, Giuseppe Raso, Li Liu

3:51 Paper **431b**: Characterization of Vortex Formation and Blend Time in Unbaffled Tanks

— **Robert P. Hesketh**, Arthur W. Etchells III, Christopher O'Connell, Nicholas Tiwari, Anthony Salemo

4:12 Paper 431c: Suspension of Large and Dense Particles in Stirred Vessels: Further Application and Validation of Grenville-Mak-Brown (GMB) 2015 Approach

— **Jason J. Giacomelli**, Richard K. Grenville, Harry E.A. Van den Akker

4:33 Paper **431d**: An Improved Kinetic Model for Micromixing Characterization Using the Villermaux-Dushman Method — *Arturo N. Manzano Martinez,* Sander Haase, Melissa Assirelli, John van der Schaaf

4:54 Paper **431e**: Comparison of CFD Simulations to Experimental Results for Blend Time of Turbulent Newtonian Fluids in Stirred Tanks

— **Aaron Strand**, John A. Thomas

5:15 Paper 431f: Comparison of Blend Time Measurements: An Experimental and Computational Study

— **Eric E. Janz**, Kevin Myers, Nicholas A Brown

5:36 Paper **431g:** Controlled Droplet Size for Oil-in-Water Emulsions: Experimental and Modeling Approach to Characterize Work History Applied By Mixing Devices

— **Margaret Y. Hwang**, Chang Kai Wu, Sarat Chandra Kuchibhatla

(432) Workshop on Utilizing Leadership Advisory Boards (aka Master Minding)

Tuesday, Nov 12, 3:30 PM Hyatt Regency Orlando, Bayhill 19 Teresa A. Jurgens-Kowal, Chair

Sponsored by: Professional Development

3:30 Paper 432a: Part 1 – Applying Creativity Tools

— Teresa A. Jurgens-Kowal

4:45 Paper 432b: Part 2 – Practicing Master Minding

— Teresa A. Jurgens-Kowal

5:15 Paper 432c: Part 3 – Setting & Achieving Goals

— Teresa A. Jurgens-Kowal

(433) Ammonia Cracking Tuesday, Nov 12, 4:00 PM Hyatt Regency Orlando, Regency

Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

4:00 Paper **433a**: Carbon-Free H₂ Production from NH₃ Triggered at Ambient Temperature with Oxide Supported Ru Catalysts

— **Katsutoshi Nagaoka**, Katsutoshi Sato, Yuta Ogura

4:23 Paper 433b: Material Discovery and Investigation of Novel Y Containing Ru Catalysts for Low Temperature Ammonia Decomposition

— **Katie McCullough**, Travis Williams, Jochen Lauterbach

4:46 Paper 433c: High Flow Ammonia Cracking between 400 - 600C — Adam Welch, Jonathan Kintner, Christopher Cadigan, Ryan O'Hayre, Joseph Beach

5:09 Paper 433d: Ammonia Decomposition and Separation Using Catalytic Membrane Reactors
— Stephen N. Paglieri, Aadesh X. Harale, Aqil Jamal, **Sai P. Katikaneni**, Toshiaki Matsui, Hiroki Muroyama,

(434) SBE's James E. Bailey Award

Tuesday, Nov 12, 6:00 PM Hyatt Regency Orlando, Regency Ballroom V

Koichi Eguchi

Sponsored by: Awards Committee

6:00 Paper **434a:** Systems Biology of Metabolism: Role in Production of Advanced Biofuels, Obesity and Cancer — Jens Nielsen

(435) Poster Session: Ammonia Energy

Tuesday, Nov 12, 6:00 PM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

Paper 435a: Boosting Ammonia Synthesis in NH₃-Sieving Inorganic Membrane Reactor

— **Huazheng Li**, Surya Padinjarekutt, Shenxiang Zhang, Ji Jiang, Fanglei Zhou, Qiaobei Dong, Miao Yu

Paper 435b: Activation By High Temperature Reduction of Ru Catalyst Supported on Rare Earth Oxide for Ammonia Synthesis

— **Yuta Ogura**, Katsutoshi Nagaoka, Katsutoshi Sato

Paper 435c: Electrochemical Promotion of Ammonia Synthesis with Proton-Conducting Ceramic Fuel Cells -Function of Electrode Interface for Ammonia Formation Reaction-

— **Junichiro Otomo**, Chien-l Li, Kazunori Yamamoto, Hiroki Matsuo Paper 435d: Ammonia Generation By Low Energy Electrical Corona Discharge Processes

— **Yu Miao**, Alexandre Yokochi, Annette von Jouanne, Ryan Collin

Paper 435e: In Situ Growth of Nitrogen-Doped Carbon Coated γ-Fe₂O₃ Nanoparticles on Carbon Fabric for Electrochemical N₂ Fixation — Yan Li, Yang Hou

Paper 435f: Electrochemical Reduction of Dinitrogen to Ammonia Using Different Morphologies of Copper As

— **Nishithan C. Kani**, Meenesh R. Singh

Paper 435g: Electrochemical H₂-Membrane Reactor for NH₃ Synthesis from N₂ and H₂O By Electricity Using Ru Catalyst, Pd Membrane Cathode, Phosphate Electrolyte, and Pt Anode at 250°C

— **Jun Kubota**, Kanako Imamura

Paper 435h: Synthesis of Ammonia By RF Non-Thermal Plasma over Ni-MOF-74

- Maria Carreon

Electro Catalysts

Paper 435i: Ocean Thermal Energy Ammonia Production and Heat Transport to Reverse Global Warming

— Paul Curto

Paper 435j: Ammonia Production Can be Practically Free

— David Judbarovski

Paper 435k: Proton-Based Solid Acid for Ammonia Removal

— **Masakuni Yamaguchi**, Tomoyuki Ichikawa, Hikaru Miyaoka, Keita Nakajima, Tengfei Zhang, Hiroki Miyaoka, Yoshitugu Kojima

Paper 435I: Analysis of an Ammonia/ Ammonium Nitrate Fuel's Thermal Decomposition By Mass Spectrometry and Thermogravimetric Analysis

— **Bar Mosevitzky**, Gennady E. Shter, Gideon S. Grader

(436) Ammonia Synthesis: Decarbonizing Hydrocarbon Feedstocks and Fuels

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

8:00 Introductory Remarks

8:03 Paper 436a: Reducing the Carbon Footprint of Ammonia As Green Energy Carrier

- Matteo Masanti

8:26 Paper 436b: Biomass Based Sustainable Ammonia Production — *Antonio Sánchez, Mariano Martín, Pastora Vega*

8:49 Paper 436c: Simulation of an Ammonia Plant Integrated with the Allam Cycle for Commercial Production of Ammonia and Power

— **Song Wang**, Dan Fernandes, Qiang Xu, Daniel Chen

9:12 Paper 436d: The Role of Carbon Capture and Storage Incentives in Ammonia Fuel Production

— **Mike Fowler**, Jonathan Lewis

9:35 Paper 436e: Monolith Materials: Ammonia Production from Natural Gas Using Pyrolysis

- Tim Rens, Rob Hanson

(437) 3D Printing of Functional Materials

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 28 Nese Orbey, Chair Nune Satish, Co-Chair

Sponsored by: 3D Printing

8:00 Introductory Remarks

8:05 Paper 437a: Fused Filament Fabrication (FFF) and Functional Materials

- Michael E. Mackay

8:40 Paper 437b: Inkjet-Based 3D Printing of Functional Materials

— Kavin Kowsari, Shing-Yun Chang, **Anson Ma**

9:05 Paper **437c:** A Biocompatible Conductive Ink for 3D Printing of Flexible Electronics

— Amir A. Kazemzadeh Farizhandi, Shahrouz Zamani Khalajabadi, Iman Noshadi, Vaishali Krishnadoss

9:22 Paper **437d**: 3D Printed Reconfigurable Liquid Crystal Elastomers Via Light-Triggered Dynamic-Coyalent Bonds

- Emily Davidson

9:39 Paper 437e: Expanding Membrane Functionality through Additive Manufacturing

— **William A. Phillip**, John R. Hoffman, Feng Gao

9:56 Paper 437f: Additive Manufacturing of Mechanically Adaptive Polymer / Nanocellulose Composites

— **Michael J. Bortner**, Earl J. Foster, Jacob Fallon

10:13 Paper 437g: Material Selection and Formulation for Material Extrusion Additive Manufacturing

— Tone D'Amico, Masoumeh Pourali, Amy M. Peterson

(438) Advances in Biosynthesis: Chemi-Enzymatic Conversion

Wednesday, Nov 13, 8:00 AM
Hyatt Regency Orlando, Celebration 4
Hyunmin Yi, Co-Chair
Jason T. Boock, Co-Chair
Qing Sun, Co-Chair

Sponsored by: Bioengineering

8:00 Paper **438a**: Novel Acyloin Condensation Reaction Enables One-Carbon Bioconversion

— **Alexander Chou**, James M. Clomburg, Shuai Quan, Ramon Gonzalez **8:18** Paper **438b**: Development of a Novel Cooperative Photoenzymatic System for Stereoconvergent Reduction of C=C without Co-Factor Regeneration — *Yajie Wang*, *Lam Vo*, *Xiaoqiang Huang*, *Huimin Zhao*

8:36 Paper 438c: Enantioselective Synthesis of (S)-1,2,3,4- Tetrahydroisoquinoline Carboxylic Acids Via D-Amino Acid Oxidase Mediated Chemo-Enzymatic Cascade Reaction — Shuyun Ju, Yayun Liu, Gang Xu, Jianping Wu, Lirong Yang

8:54 Paper **438d**: Upgraded Bioelectrocatalytic N₂ Fixation: From N₂ to Chiral Amine Intermediates

— *Hui Chen, Shelley D. Minteer*

9:12 Paper 438e: Multi-Enzymatic Cascade Reactions with Integrated Separation in a Complex 2-Phase

System

— Jens Johannsen, Claudia

Engelmann, Andreas Liese, Georg Fieg,
Paul Bubenheim, Thomas Waluqa

9:30 Paper 438f: Expanding Whole Cell Catalysis Using Extracellular Flectron Transfer

— Gang Fan, Christopher M. Dundas, Austin J. Graham, **Benjamin K. Keitz**

9:48 Paper 438g: Invited Speaker - Advances in Biosynthesis

- David Nielsen

(439) Advances in Catalysis for Syngas Production

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Challenger 41/42

Dushyant Shekhawat, Chair Daniel J. Haynes, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

8:00 Paper **439a**: Effect of Synthesis Methods on Dry Reforming of Methane over Ni/Ce_Zr,-XO,

— **Yimeng Lyu**, Jennifer Jocz, Rui Xu, Carsten Sievers

8:18 Paper 439b: Carbon Tolerant Nickel Based Pyrochlores for Low S/C Methane Reforming: Effect of La

— **Daniel J. Haynes**, Yan Zhou, Amy Falcon, Dushyant Shekhawat, James J. Spivey

8:36 Paper 439c: Reforming of Methane over Ni and Ca Based Pyrochlore Catalysts to Produce Syngas — Srikar Bhattar, Swarom Kanitkar, Ashraf Abedin, Dushyant Shekhawat, Daniel J. Haynes, James J. Spivey

8:54 Paper 439d: Hydrogen Generation Using Heavy Oil Feedstocks — Girish Srinivas, Steven Schwab, Harsha Vempati, Brian Gebhard, Steven Gebhard

9:12 Paper 439e: Deactivation of Unsupported and Silica-Supported Cobalt Nanoparticles for Ethanol Steam Reforming and CO₂ Methanation — Paola Riani, Gabriella Garbarino, Tullio Cavattoni, Guido Busca **9:30 Paper 439f:** Toluene Reforming Using Nickel Based Catalysts Made from Mining Residues

— **Salma Belbessai**, Esma Ines Achouri, Nicolas Abatzoglou

9:48 Paper **439g**: Low Temperature Steam Methane Reforming Using Lanthanides Modified Ni/Al₂O₃ Catalyst for Hydrogen Production for Fuel Cells — *Shakeel Ahmed, Sai P. Katikaneni, Aadesh X. Harale*

10:06 Paper 439h: Autothermal (CO₂ and O₂) Di-Reforming of Methane with the Ni-UGSO Catalyst: Lab-Scale Results and Kg-Lab Scale Tests at Industrial H₂ Production Conditions

— **Nicolas Abatzoglou**, Frank Dega, Mostafa Chamoumi

(440) Advances in Fluid Particle Separations

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Coral Spring I/II Isaac K. Gamwo, Chair Seyi Odueyungbo, Co-Chair

Sponsored by: Fluid-Particle Separations

8:00 Paper 440a: Modeling of Particle Retention and Penetration Depth in Deep Bed Filtration

— Siying Zhang, J. J. McCarthy

8:20 Paper 440b: Methods to Study Influence of Surfaces in Crystallization Processes: Scaling and Supersaturation Depletion

— Sankaranarayanan Ayyakudi Ravichandran, Jacob Hutfles, John Pellearino

8:38 Paper 440c: Electrocoalescence of an Aqueous Drop at Water-Oil Interface

— **Vikky Anand**, Vinay Juvekar, Rochish Thaokar

8:56 Paper 440d: Effect of Glycine Pre-Leaching of Copper- Gold Bearing Low Grade Ore Prior to Cyanidation

— Tafirenyika Chiyanike, Chidochashe K. Siyavora, **Nkosikhona Hlabangana**

9:14 Paper 440e: Main Operating Parameters of the Spouting Regenerator for the Collecting Particles of the Moving Bed Filter

— **Ming Chang**, Sihong Gao, Yiping Fan, Chunxi Lu

(441) Advances in Process Intensification

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 17 Chongwei Xiao, Chair Jayachandran Devaraj, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

8:00 Paper **441a**: Process Intensification: A Novel Approach for Development of Smaller, Cleaner and Energy Efficient Technologies

— Sirshendu Guha

- **8:20 Paper 441b:** Process Intensification Via Batch-to-Continuous Transition in the Production of Lubricants
- **Nasser Al Azri**, Edmund Sam-Gyandoh, Hari C. Mantripragada, Corey Clifford, Robert M. Enick, Cliff Kowall, Götz Veser
- **8:40** Paper **441c:** Process Intensification Framework for Extractive Separation Systems
- **Yuhe Tian**, Iosif S. Pappas, Styliani Avraamidou, Efstratios N. Pistikopoulos
- 9:00 Paper 441d: A Modified Mixed-Acid Catalytic System for Beckmann Rearrangement of Cyclohexanone Oxime in a Microreactor
- **Chencan Du**, Jisong Zhang, Liantang Li, Guangsheng Luo
- **9:20 Paper 441e:** Fast Pyrolysis of Pine Biomass in a Gas Solid Vortex Reactor
- **Manuel Nunez Manzano**, Arturo Gonzalez Quiroga, Shekhar Kulkarni, Chitrakshi Goel, Guy B. Marin, Geraldine J. Heynderickx, Kevin M. Van Geem
- **9:40** Paper 441f: Synthesis of Optimal Hybrid Separation Processes *Salih E. Demirel, Shachit S. Iyer,*
- Sain E. Demirei, Snachii S. Iyer, Jianping Li, Anjan Kumar Tula, Mario Richard Eden, Rafiqul Gani, M. M. Faruque Hasan
- **10:00** Paper **441g**: Multi-Objective Optimization of Forced Periodic Processes Using Nonlinear Frequency Response Method
- Luka Zivkovic, Viktor Milic, Menka Petkovska
- (442) Advances in Supply Chain Design and Logistics

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 25 Chrysanthos E. Gounaris, Chair Zhang Qi, Co-Chair

Sponsored by: Computers in Operations and Information Processing

- **8:00** Paper **442a**: Supply Chains with Modular and Mobile Production Units: Optimization Framework and Solution Methods
- Andrew Allman, Qi Zhang
- **8:19** Paper **442b:** A Branch-and-Cut Algorithm for Continuous-Time Inventory Routing Problems
- **Akang Wang**, Xiandong Li, Chrysanthos E. Gounaris
- 8:38 Paper 442c: A Novel Framework for Shale Gas Supply Chain Network Considering MPC-Based Pumping Schedule of Hydraulic Fracturing in Unconventional Reservoirs
- **Yuchan Ahn**, Prashanth Siddhamshetty, Kaiyu Cao, Joseph Sang-Il Kwon
- **8:57** Paper **442d**: Enabling Precision Healthcare through Patient-Centric Supply Chain Networks
- **Maria M. Papathanasiou**, Matthew Lakelin, Nilay Shah

- **9:16** Paper **442e**: Effect of Flexible Delivery Windows during Multi-Period Vehicle Routing
- **Aliakbar Izadkhah**, Anirudh Subramanyam, José Miguel Laínez-Aguirre, Jose M. Pinto, Chrysanthos E. Goungris
- **9:35 Paper 442f:** A Market Clearing Framework for the Evaluation of Municipal Waste Management and Recycling Economies
- Philip Tominac, Victor M. Zavala
- **9:54** Paper 442g: Closed-Loop Optimal Operational Planning of Supply Chains with Product Quality Dynamics
- Fernando Lejarza, Michael Baldea
- **10:13 Paper 442h:** Estimation of Marginal Cost to Serve Individual Customers
- **Akang Wang**, Jeffrey E. Arbogast, Gildas Bonnier, Chrysanthos E. Gounaris

(443) Applications of Data Science in Catalysis and Reaction Engineering II

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Peacock Spring

Zachary Ulissi, Chair Srinivas Rangarajan, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

- **8:00** Paper **443**a: An Automated Job Management Framework for High Fidelity Quantum Chemistry Calculations
- **Sai Krishna Sirumalla**, David Farina Jr., Nathan Harms, Richard H. West
- **8:18** Paper 443b: Theoretical Investigation of Pt-Catalyzed Dehydrogenation of Propane to Propylene: Applying Uncertainty Analysis to Reaction Kinetics
- Charles Fricke, Andreas Heyden
- **8:36 Paper 443c:** Symbolic Regression for the Automated Physical Model Identification in Reaction Engineering
- **Liwei Cao**, Pascal Neumann, Danilo Russo, Vassilios S. Vassiliadis, Alexei A. Lapkin
- 8:54 Paper 443d: A Machine Learning Based Algorithm for Rate Estimation
- **Matthew S. Johnson**, William H. Green
- **9:12** Paper **443e**: Using Data Driven Models to Gain Insight on Spin- and Oxidation-State Dependent Behavior of Reaction Energetics for Light Alkane Oxidation
- **Aditya Nandy**, Jon Paul Janet, Chenru Duan, Heather J. Kulik
- **9:30 Paper 443f:** Statistical-Learning-Assisted First-Principles Modeling of Catalysts Sintering
- **Yifan Wang**, Ya-qiong Su, Emiel Hensen, Dionisios G. Vlachos
- **9:48** Paper 443g: Data-Driven Strategy for Ab-Initio Microkinetic Modeling of C₁-Reaction on Copper (111) from Disparate Experimental Datasets
- **Huijie Tian**, Srinivas Rangarajan

10:06 Paper 443h: Generalized Brønsted Evans Polanyi Relationships for Metal Surfaces from Machine Learning

- Florian Göltl, Manos Mavrikakis

(444) Applied Math for Biological and Biomedical Systems

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 26 Ashlee N. Ford Versypt, Chair Roman Voronov, Co-Chair Ravendra Singh, Co-Chair Elizabeth Read, Co-Chair Stacey D. Finley, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

- **8:00 Paper 444a:** Optfill: A Novel Optimization-Based Tool to Automate the Gapfilling of Genome-Scale Metabolic Models
- Wheaton Schroeder, Rajib Saha
- **8:18** Paper 444b: Fast Uncertainty Quantification in Dynamic Flux Balance Analysis Models Using Sparse Multi-Element Polynomial Chaos
- **Joel Paulson**, Marc Martin-Casas, Ali Mesbah
- **8:36** Paper 444c: Genome Scale Model Analysis of *Clostridium Tyrobutyricum* for Butyl Butyrate Production
- **Kiumars Badr**, Jie Zhang, Yi Wang, Jin Wang
- **8:54** Paper 444d: Kinetic Model for the Enzymatic Synthesis of Galacto-Oligosaccharides: Describing Galactobiose Formation
- Guilhermina Schultz, Ronald Alexander, Fernando V. Lima, Roberto C. Giordano, **Marcelo P. A. Ribeiro**
- **9:12 Paper 444e:** Agent-Based Modeling of the Effects of Colony Size and Neonicotinoid Exposure on Bumblebee Behavior within Nests
- **Ashlee N. Ford Versypt**, James D. Crall, Benjamin L. de Bivort, Biswadip Dey
- **9:30 Paper 444f:** A Dynamical Systems Approach to Modeling the Inflammatory Response in Sepsis
- **Brian McLaverty**, Gilles Clermont, Robert S. Parker
- **9:48** Paper **4449**: Do Comorbid Medical Conditions Affect Autism Spectrum Disorder Diagnosis Via Big Data Analysis of Plasma Metabolites?

 Troy Vargason, Emily Roth,
- Genevieve Grivas, Richard E. Frye, Juergen Hahn
- 10:06 Paper 444h: Image-Based Mass Transport Simulation Shows How to Optimize Tissue Engineering Scaffold Architecture for Optimal Oxygen and Nutrient Transport
- **Thanh Danh Nguyen**, Olufemi Kadri, Cortes Williams III, Vassilios I. Sikavitsas, Roman Voronov

(445) Atmospheric Chemistry and Physics: Laboratory Studies Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Blue Spring I/II Shunsuke Nakao, Chair Kristina Wagstrom, Co-Chair Marwa El-Sayed, Co-Chair

Sponsored by: Air

8:00 Paper 445a: Light Scattering from Soot Nanoparticle Agglomerates — Georgios A. Kelesidis, Mohammad Reza Kholghy, Joel Zuercher, Julian Robertz, Martin Allemann, Aleksandar Duric, Sotiris E. Pratsinis

8:20 Paper 445b: The Role of Organic Solvents in Cholestrol Cloud Condensation Nuclei Activation
— Farima Barati, Akua Asa-Awuku

8:40 Paper 445c: Role of Polarity Distribution of Organics in Aerosol Hygroscopicity

— **Shunsuke Nakao**, Vikram Pratap, Aditya Srikakulapu

9:00 Paper 445d: Estimation of Vapor Wall-Loss in Smog Chamber Experiments

— **Kerrigan Cain**, Eleni Karnezi, Spyros N. Pandis

9:20 Break

9:40 Paper 445f: Insight into the Mechanism of Alkali Resistance over Cunbti Catalyst for the Selective Catalytic Reduction of NO_x with NH₃ — Su-Jing Li, Xiaoxiang Wang, Wei Li

10:00 Paper 445g: Efficient Removal of SO₂ and NO_x from Flue Gas Using Yellow Phosphorus and Phosphate Slurry As Adsorbent

— Dedong He**, Yi Mei**, DeLong Xie, Yuanzhi Zhu, Xinzhi Chen, Yanping He

(446) Catalysis for Nitrogen Chemistry I: Electrocatalytic Nitrogen Reduction

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom D Andrew Medford, Chair Jingjie Wu, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper 446a: When Metal Meets Boron: Cooperative Catalysis for High Efficiency Electro-Synthesis of Ammonia *Jianfang Zhang*, *Yujing Tian*, *Jingjie Wu*
- **8:18** Paper 446b: Transition Metal Nitrides Catalyzed Electrochemical Nitrogen Reduction Reaction

 Bingjun Xu, Xuan Yana, Jared Nash
- **8:36 Paper 446d:** Pd-Catalyzed Electrohydrogenation of Dinitrogen to Ammonia
- Xiaofeng Feng

- 8:54 Paper 446e: Proton Control in Electrochemical Ammonia Synthesis
- **Matteo Cargnello**, Jay Schwalbe, Aayush R. Singh, Brian A. Rohr, Michael Statt, Adam Nielander, Joshua M. McEnaney, Suzanne Andersen, Viktor Colic, Ib Chorkendorff, Thomas F. Jaramillo, Jens K. Norskov
- 9:12 Paper 446f: Promoting Reliable Electrocatalytic N₂ Reduction
 Adam Nielander, Joshua M.
 McEnaney, Jay Schwalbe, Sarah Blair,
 Jonathan G. Baker, Thomas F. Jaramillo
- **9:30 Paper 446g:** Continuous Lithium-Mediated Ammonia Synthesis at Ambient Conditions
- **Karthish Manthiram**, Nikifar Lazouski, Zachary Schiffer, Kindle Williams
- **9:48** Paper 446h: A Rotating Ring Disk Electrode Investigation of Oxides for Photocatalytic Nitrogen Fixation
 Marta Hatzell, Yu-Hsuan Liu
- 10:06 Paper 446i: Discussion of
- protocols for measuring ammonia

 Andrew Medford

(447) Cells, Organs, and Labs on a Chip: Tissue Microenvironments

Wednesday, Nov 13, 8:00 AM
Hyatt Regency Orlando, Celebration 2
Ryan Koppes, Chair
Heather Fahlenkamp, Co-Chair
Adriana San-Miquel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **8:00** Paper 447a: Migration of Artificially Activated B Cells in a Microfluidic Device-Induced CXCL-12 Gradient
- Rachel Stokes, Kyung-Ho Roh
- **8:18** Paper 447b: A Liver on a Chip Model Mimicking the Intrahepatic Bile Duct
- **Amin Vossoughi Shahvari**, Olivia Cali, Howard W. T. Matthew
- **8:36** Paper 447c: A Microscale, Full-Thickness, Human Skin on a Chip Assay Simulating Neutrophil Responses and Antibiotic Treatment to Skin Infection
- **Jae Jung Kim**, Felix Ellett, Carina N. Thomas, Fatemeh Jalali, R. Rox Anderson, Daniel Irimia, Adam B Raff
- **8:54 Paper 447d:** Neuro-Cardiac Axis on a Chip: Neural Remodeling of the Cardiac Microenvironment
- **Jonathan Soucy**, Tess Torregrosa, Sanjin Hosic, Sebastian Moreno Arteaga, Abigail Koppes, Ryan Koppes
- **9:12** Paper 447e: Noninvasive Manipulation of Cells and Chemicals within Live Cultures Via Addressable Microfluidics
- Anh Tong, Long Quang Pham, Vatsal Shah, Paul Abatemarco, Roman
- **9:30** Paper 447f: Developing Islet-on-a-Chip Using Human Pluripotent Stem Cells *Connor Wiegand, Xiang Li, Lans Taylor, Ipsita Banerjee*

9:48 Paper 447g: Body-on-a-Chip Systems for Drug Development — *Ying Wang, Michael Shuler*

(448) Chemical Looping Processes Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Regency

Ballroom Q
Andrew Tong, Chair
JoAnn S. Lighty, Co-Chair
Douglas Straub, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

- **8:00 Paper 448a:** Recent Progress on Key Technical Barriers for Chemical Looping Combustion
- **Douglas Straub**, Justin Weber, Samuel Bayham
- 8:21 Break
- **8:42** Paper 448c: Particle Properties in Techno-Economic Analysis of Chemical Looping Hydrogen Generation
- Yitao Zhang, Fanhe Kong, Andrew Tong
- 9:03 Paper 448d: High-Purity Hydrogen from Biogas with a Combined Reformer and Fixed-Bed Chemical Looping System
- **Sebastian Bock**, Robert Zacharias, Karin Malli. Viktor Hacker
- **9:24** Paper 448e: Perovskite Oxygen Sorbents for "Low Temperature" Thermochemical Air Separation: Correlating Compositions with Redox Performance
- **Emily Krzystowczyk**, Jian Dou, Xijun Wang, Fanxing Li
- **9:45** Paper 448f: MoVNbTeO for Chemical Looping Oxidative Dehydrogenation of Ethane
- **Samuel Gabra**, Stuart A. Scott, Gareth Williams, Stephen Poulston, John S. Dennis
- $\begin{array}{ll} \textbf{10:06 Paper 448g:} & \text{Improving Fe}_2 O_3 \\ \text{Reactivity with CO and CH}_4 & \text{in Chemical Looping Systems By Low Percentage} \\ \text{1st-Row Transition Metal Dopants: A} \\ \text{Theoretical and Experimental Work} \\ \end{array}$
- **Yu-Yen Chen**, Mengqing Guo, Yan Liu, Liang-Shih Fan

(449) Chemical Transformations of Lignocellulosics to Fuels and Nanomaterials

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Discovery 47 Maobing Tu, Chair Yaseen Elkasabi, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

- **8:00 Paper 449a:** Desulfurization and Coking of Hydrocarbon Fractions from Biomass Pyrolysis Oils
- Yaseen Elkasabi

- **8:25** Paper **449b:** Investigation of the Effect of Wet Flue Gas on Torrefaction of Corn Residues Pellets in a Fixed Bed Reactor
- Onsree Thossaporn, Tippayawong Nakorn, Travis Williams, Katie McCullough, Elizabeth Barrow, Ravindra Pogaku, Jochen Lauterbach
- **8:50 Paper 449c:** Mild Alkaline Pretreatment for Isolation of Native-like Lignin and Lignin-Containing Cellulose Nanofibers (LCNF) from Crop Waste
- Xuran Liu, **Yanding Li**, Chinomso Ewulonu, John Ralph, Feng Xu, Qilin Zhang, Min Wu, Yong Huang
- **9:15 Paper 449d:** Preparation of Nanofibrillated Biomass (NFB) for Thin Films and Composites
- **Samarthya Bhagia**, John Dunlap, Rick Lowden, Wellington Muchero, Yunqiao Pu, Arthur J. Ragauskas
- **9:40 Paper 449e:** Tailoring Lignin Chemistry to Manufacture Quality Material for Sustainable and Viable Biorefienry
- Joshua Yuan

(450) Colloidal Dispersions Wednesday, Nov 13, 8:00 AM

Hyatt Regency Orlando, Plaza International Ballroom K Carlos Silvera Batista, Chair Mark Kastantin, Co-Chair Yoonjee Park, Co-Chair

Sponsored by: Interfacial Phenomena

- **8:00 Paper 450a:** Mapping Evanescent Wave Scattering Form Anisotropic Particles
- Aidin Rashidi, Adrian Doicu, Alina A. Vasilyeva, Dmitry S. Efremenko, Thomas Wriedt, **Christopher L. Wirth**
- **8:15 Paper 450i:** Analytical Ultracentrifugation Based Quantification of the Packing Density of Linear Alkanes Inside ~1.5 Nm Diameter Single-Wall Carbon Nanotubes
- Jeffrey A. Fagan
- **8:30 Paper 450c:** Solvent Absorbent Amphiphilic Microgels for Pickering Emulsions
- **Bobby Haney**, Subramanian Ramakrishnan
- 8:45 Break
- 9:00 Paper 450e: The Effect of Flow and Interaction Strength on the Microstructure and Properties of a Model Carbon Black Suspension

 Julie B. Hipp, Norman J. Wagner,
- **9:15** Paper **450f**: Probe Rheology Molecular Simulations of Nanocolloidal Suspensions
- Dinesh Sundaravadivelu Devarajan, Rajesh Khare

Jeffrey J. Richards

- **9:30 Paper 450g:** Time-Concentration Superposition in Colloids Near to the Putative Glass Transition
- Gregory B. McKenna, Xiaoguang Peng, Jialun Wang, Qi Li, Dongjie Chen, Roseanna N. Zia

- **9:45** Paper **450h**: Structure and Interaction of Solvent-Free Bidisperse Polymer Brushes Investigated Using Mean-Field Theory and Molecular Simulations
- Ching-Heng Tai, Yi-Yan Zhang, **Hsiu-Yu Yu**
- **10:00 Paper 450b:** Influence of Nano and Microconfinement on Internanoparticle Interactions in Geocolloidal Dispersions
- **Yuanzhong Zhang**, Younjin Min, Stephen Merriman

(451) Continuous Processing Technologies Applied in Drug Product Manufacturing

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 7 Nima Yazdanpanah, Chair Dimitrios I. Gerogiorgis, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **8:00** Paper **451a:** Economic Evaluation Tool for Holistic Design of Solid Drug Product Manufacturing Processes Considering Continuous Technology
- **Kensaku Matsunami**, Fabian Sternal, Keita Yaginuma, Shuichi Tanabe, Hiroshi Nakagawa, Hirokazu Sugiyama
- **8:19 Paper 451d:** Advanced Quality Control Method for a Continuous Wet Granulation Tableting Line
- Manuel Kreimer, Jakob Rehrl, Stephan Sacher, Valjon Demiri, Anna Peter, Wen-Kai Hsiao, Johannes G. Khinast
- **8:38 Paper 451e:** Investigating Effects of Dynamic Process Variability in Continuous Direct Compression on Tablet Quality Attributes through a Science-Based Digital Twin
- **Dana Barrasso**, Xin Li, Sean K. Bermingham, Gavin Reynolds
- **8:57 Paper 451f:** Use of Blue Dye Powder Tracer to Evaluate the Residence Time Distribution of Continuous Manufacturing Direct Compression Equipment
- William E. Engisch Jr., Michael T. Kennedy, Steve La
- **9:16 Paper 451g:** Transient Mean Age Analysis in Continuous Processing Systems
- John A. Thomas
- **9:35 Paper 451h:** Product Robustness within a Dry Granulation Continuous Manufacturing Line
- **Steven Dale**, Marcus O'Mahony, Pongpumin Bunchatheeravate, Greg Connelly
- 9:54 Paper 451b: Impact of Material Properties and Process Parameters on Residence Time Distributions in Pilot Scale Continuous Powder Blending Scott M. Krull, Celia N. Cruz, Thomas O'Connor

10:12 Paper **451c**: Residence Time Distribution Determination and Prediction with Discrete Element Method (DEM) in Continuous Blending Processes

— **Nima Yazdanpanah**, Scott M. Krull, Celia N. Cruz, Thomas O'Connor

(452) Cybersecurity

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 27 Helen Durand, Chair Joseph Sang-II Kwon, Co-Chair

Sponsored by: Next-Gen Manufacturing

8:00 Paper 452a: Cyber-Security with Dynamic Watermarking for Process Control Systems

— **Jaewon Kim**, Woo-Hyun Ko, P. R. Kumar

8:19 Paper 452b: Simultaneous Analysis of Control and Cyberattack Detection Algorithms for Enhanced Operational Safety

— Matthew Wegener, Helen Durand

8:38 Paper 452c: Cybersecurity of Process Control Systems Via a Two-Tier Control Architecture

— Zhe Wu**, Scarlett Chen**, Mohammed Alhajeri, Panagiotis D. Christofides

8:57 Paper 452d: A Model-Based Approach for the Analysis and Mitigation of Cyber-Attacks in Networked Process Control Systems

— Amr Zedan, Nael H. El-Farra

9:16 Paper 452e: On the Intersection of Process/Equipment Design and Control System Cybersecurity

– Helen Durand

9:35 Paper 452f: Cyber-Physical Security of Advanced Automated Continuous Pharmaceutical Manufacturing Pilot-Plant — Ravendra Singh

9:54 Paper 452g: Keynote Talk: Cybersecurity for the Power Grid — *Steve Chapin*

(453) Department Heads Forum (Invited Talks)

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 22 Valerie L. Young, Chair Edward Maginn, Co-Chair

Sponsored by: Department Heads Forum

8:00 Welcoming Remarks

8:05 Salary Survey Report

8:25 ABET update

8:45 Break

9:05 Further programming to be announced

10:25 Concluding Remarks

(454) Diffusion, Transport, and Dynamics in Adsorption Systems

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Manatee Spring II

T. Grant Glover, Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 454a: Diffusion Measurements Using a Volumetric Differential Pressure Apparatus

— Jinyu Wang**, Enzo Mangano**, Stefano Brandani

8:21 Paper 454b: Anomalous Relationship between Molecular Size and Diffusivity in ZIF-11 By a Combined Application of Diffusion NMR, Volumetric Adsorption Method, and IR Microscopy

— Amineh Baniani, Christian Chmelik, Evan M. Forman, Lei Fan, Kirk J. Ziegler, Erkang Zhou, Fengyi Zhang, Richelle Lyndon, Ryan Lively, Sergey Vasenkov

8:42 Paper **454c:** Impact of MOF Pore Size on the Diffusion of CWA Simulants — *Trenton M. Tovar, Christopher Karwacki, John J. Mahle*

9:03 Paper 454d: Integrating Material and Process Design for Kinetic Separation

— **Trisha Sen**, Yoshiaki Kawajiri, Matthew Realff

9:24 Paper 454e: Characterization of Sorption Kinetics of CO₂ from N₂-Rich Gas Mixtures Studied By Breakthrough Experiments on Zeolites

— Andreas Möller, Robert Eschrich, Christian Reichenbach

(455) Division Plenary: Materials Engineering & Sciences Division (Invited Talks)

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 5 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 **455a**: Polymer Hydroxide Exchange Membrane Fuel Cells for Affordable Zero-Emission Vehicles

— Yushan Yan

8:40 Owens-Corning Award Introduction

8:45 Paper **455b**: Bigsmiles: A Text-Based Representation for Polymer Structure

— **Bradley D. Olsen**, Tzyy-Shyang Lin, Connor W. Coley, Hidenobu Mochigase, Klavs F. Jensen

9:15 Paper 455c: In Search of the Photonic Band Gap

— **Sharon C. Glotzer**, Rose Cersonsky, James Antonaglia, Bradley Dice

9:40 Paper **455d**: Fabrication of Nano-Structured Catalyst Supports by ALD

— Raymond J. Gorte **10:05** Paper **455e:** Making Complex Materials out of Simple Particles – Strategies for Particle Assembly, Binding and Manipulation in Magnetic Fields and in Multiphasic Systems

- Orlin D. Velev

10:30 Concluding Remarks

Stefan Radl, Co-Chair

(456) Dynamics and Modeling of Particulate Systems: Applications Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 21 Kuochen Tsai, Chair

Sponsored by: Solids Flow, Handling and Processing

8:00 Paper 456a: Predicting Critical Outlet Width of Hopper Systems Using Finite Element Analysis

— Kunal S. Pardikar, Carl R. Wassgren

8:18 Paper **456b**: The Dynamics of Sphere-Rod Mixtures Evacuating Wedge Hoppers

- Aaron Lattanzi, Jonathan J. Stickel

8:36 Paper **456c:** Computational and Experimental Studies of Mechanical Compression of Flexible Fiber Packings — *Qingzhao Liu, Yanjie Li, Dandan Xu, Yu Guo, Carl Wassgren, Jennifer Sinclair Curtis*

8:54 Paper 380ax: Modeling Particle-Induced Turbulence Using Sparse Regression with Embedded Invariance

— **Sarah Beetham**, Jesse Capecelatro

9:12 Paper 456d: The Discrete Element Modeling (DEM) of Eccentric Weights Based Vibratory Dryer

— **Rohit Kumar**, Subhash Thakur, Shrikant Swaminathan

9:30 Paper **456e**: Modeling Cohesive Powder Flow in a Rotating Drum Using the Finite Element Method and a Mohr-Coulomb Material Model

— **Abhishek Paul**, George Elias, Yu Liu, Marcial Gonzalez, Carl R. Wassgren

9:48 Paper **456f**: A CFD-DEM Based Model for Wet Granulation Process in a Rotary Drum

— **Amit Patil**, John Morud, Stein Tore Johansen Sr.

10:06 Paper **456g**: CFD Simulation of Particle Dissolution in Mixing Tanks — *Yujian Sun*, *Nikolaos Kladias*

(457) Effective Communication Skills for ChE

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 23 Bernard J. Van Wie, Chair Amanda Simson, Co-Chair

Sponsored by: Undergraduate Education

8:00 Paper **457a:** Practicing the ABCs of Technical Communication Using Realistic Problems and Homework Memos

— Rebecca Ong

8:18 Paper 457b: Write-to-Learn and Learn-to-Write: Using Writing in Teaching Technical Content

- Elif E. Miskioglu

8:36 Paper **457c:** Flipping Writing Revisions: Students Devise Self-Revision through Reflection in the Engineering Laboratory

— Jamie Gomez, Catherine Hubka, Vanessa Svihla, Marina Miletic, Eva Y. Chi, Abhaya K. Datye

8:54 Paper **457d:** Utilizing Peer Review to Improve the Quality of Unit Operations Assignments

- Sarah A. Wilson

9:12 Paper 457e: Communication Skills Instruction in a Two-Semester Capstone Design Course Sequence

— **Matthew L. Alexander**, Joseph Amaya

9:30 Paper 457f: Framework for Conducting a Technical Communication Crosswalk across a Chemical Engineering Curriculum

— Andrew Pfluger, Matthew Armstrong, Andrew Biaglow, Corey James, Enoch Nagelli, April Miller

9:48 Paper 457g: Theory, Design, and Early Implementation Results of a Multi-Tiered, Scaffolded Writing Pedagogy — Kitana Kaiphanliam, Olivia Reynolds, Di Wu, Olusola Adesope,

(458) Energetic Materials: Engineered Particles and Interfaces Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 20 Lori J. Groven, Chair Victor Stepanov, Co-Chair

Sponsored by: Energetics

Bernard J. Van Wie

8:00 Paper 458a: Reactive Composites of Boron and Bismuth Fluoride with Varied Fluoride Concentrations
— Siva Kumar Valluri, Mirko
Schoenitz, Edward L. Dreizin

8:12 Paper **458b**: Aluminum-Based Thermites Prepared By Staged Milling with Different Process Control Agents

— **Mehnaz Mursalat**, Mirko Schoenitz, Edward Dreizin

8:24 Paper **458c:** Electrostatic and Steric Stabilization of Nanoenergetics Suspensions

— Mouhcine Doukkali

8:36 Paper 458d: Heterogeneous Oxidation of Boron Powders and Its Role in Ignition and Combustion

— Kerri-Lee A. Chintersingh-Dinnall, Yalun Sun, Mirko Schoenitz, Edward L Dreizin

8:48 Paper 458f: Designing Composite Energetic Nanomaterials with Tunable Interfacial Activities Via Laser Ablation Synthesis in Solution

— **Dibyendu Mukherjee**, Seyyed Ali Davari, Erick L. Ribeiro, Gerd Duscher, Jennifer Gottfried

- **9:00** Paper **458g**: Boron-Based Analogs of Graphene Exfoliated from Layered Metal Diborides As Catalytic Additives to Improve the Performance of Energetic Materials
- **Harini Gunda**, Chinmay Ghoroi, Kabeer Jasuja
- **9:12** Paper **458h**: Hot-Spot Formation in Composite Energetic Materials Due to Ultrasonic and Impact Excitation As a Function of Young's Modulus and the Work of Adhesion
- **Jason Wickham**, Zane Roberts, Stephen P. Beaudoin, Steven F. Son
- **9:24 Paper 458i:** Microwave Enhancement of Boron Combustion for Solid Fuel Ramjet Applications
- Adam Lawrence, Travis R. Sippel
- **9:36** Paper **458**j: Molecular Perovskites for Energetic Applications — *Clinton Chapman*, *Lori J. Groven*
- 9:48 Paper 458k: Microwave Controlled Ignition and Combustion of an AP Composite Solid Propellant Using Graphene Oxide-Wrapped Nanoscale Thermites
- **Stuart J. Barkley**, Jordan Golberg, Keke Zhu, James B. Michael, Travis R. Sippel
- **10:00 Paper 458l:** The Microstructural Evolution and Kinetics of Thermal Decomposition of Selected Energetic Cocrystals
- Joshua Dean
- **10:12 Paper 458m:** Thermal Behavior of CL-20 at Ultra-High Heating and Cooling Rates Using Flash DSC
- **Aric Denton**, Rozana Bari, Zachary Fondren, Yung P. Koh, Victor Stepanov, Sindee L. Simon, Gregory B. McKenna

(459) Environmentally Friendly Product and Process Development for Sustainability

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 18 Qiang Xu, Chair Onkar Manjrekar, Co-Chair Deboleena Chakraborty, Co-Chair

Sponsored by: Process Research and Innovation

- **8:00 Paper 459a:** Simultaneous Product and Process Design for Tailor-Made Biofuels
- **Andrea König**, Lisa Neidhardt, Jörn Viell, Alexander Mitsos, Manuel Dahmen
- **8:21** Paper **459b:** Improving the Location Robustness of Spatially Distributed Variables for Biomass Supply Chains Under Supply Uncertainty

 Nathanial J. Cooper, Nilay Shah
- **8:42 Paper 459c:** Process Intensification in By-Product Recovery from Biobased Effluents
- Daniela Painer, Susanne Lux, **Matthaeus Siebenhofer**

- **9:03 Paper 459d:** Jet Fuels Production from Waste Cooking Oil Via Catalytic Transfer Hydrogenation
- **Elena Barbera**, Alexander Asiedu, Eleazer Resurreccion, Alberto Bertucco, Sandeep Kumar
- **9:24 Paper 459e:** The Conceptual Framework and Modeling Analysis of Compact Energy Systems
- **Sampath Gunukula**, Dat T. Tran, Ivan C. Lee
- **9:45** Paper **459f:** Synthesis and Evaluation of Dipicolinic Acid (DPA) Based Interwell Tracers for Reservoir Surveillance
- **Rena Shi**, Gawain Thomas, Sehoon Chang, Hooisweng Ow
- **10:06 Paper 459g:** Design Development of a Novel Sour Water Stripper
- Umer Zahid, Ali Al-Qadri

(460) Graphene and Carbon Nanotubes: Absorption, Separations, and Transport Processes

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Discovery 44 Ardemis A. Boghossian, Chair Geyou Ao, Co-Chair

Sponsored by: Carbon Nanomaterials

- **8:00** Paper 460a: Purification of Single-Wall Carbon Nanotubes Using Aqueous Two Phase Extraction to Single (n,m) Species in the Large Diameter Limit Han Li, Benjamin Flavel, Jeffrey A. Fagan
- **8:22** Paper 460b: A Simulation Study of the Effect of CO and CO₂ Adsorption on the Iron Particle Formation and Nanotube Nucleation for a Floating Catalyst System
- **Mauricio Carvajal Diaz**, Perla B. Balbuena
- **8:44** Paper 460c: Utilizing a Carbon Nanomaterial-Based Nanocomposite Aerogel Towards Separation and Energy Applications
- Reginald E. Rogers Jr.
- **9:06** Paper 460d: Study of Unique Kinetic Vs Thermodynamic Equilibria of Specific Chiralities of Single Walled Carbon Nanotubes
- **Aniruddha Kulkarni**, Stephen Michel, Yang Zhao, Kirk J. Ziegler
- **9:28** Paper 460e: Transformation of GO Surfaces to Reduced-GO Surfaces with Tunable Surface Chemistry and Morphology Via Pool Boiling Process *Anju Gupta*, *Aniket Rishi*, *Satish*
- **9:50 Paper 460f:** Harnessing the Intrinsic Synthesis Catalysts to Create Faradaic Carbon Nanotube Composites

Kandlikar

- Robert Emmett, Michael Kowalske, Hansen Mou, Mikaela Grady, Mark E. Poherts
- **10:12 Paper 460g:** Packaging Vertically Aligned Carbon Nanotubes into a Heat Shrink Tubing for Efficient Removal of Phenolic Pollutants
- Seung Min Moon, Chang Young Lee

(461) Heterogeneous Catalysis in Liquid Media I

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Florida Ballroom A

Omar A. Abdelrahman, Chair Alexander V. Mironenko, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00 Paper 461a:** Liquid-Phase Modeling in Heterogeneous Catalysis *Andreas Heyden*
- **8:30** Paper **461b**: Effects of Liquid Water on Selective C-O Hydrogenolysis Catalyzed By Ru-TiO₂ interfacial Sites Daniela Stück, Brian G. Frederick, Rachel Austin, Lars C. Grabow, **Thomas**
- **8:48** Paper 461c: Protic Solvents Catalyzed Synergistic H-Adatom and Proton Transfer during Methoxyphenol Hydrodeoxygenation on Ru Clusters

J. Schwartz

- **Junnan Shangguan**, Alyssa Hensley, Matthew Gradiski, Jacob Bray, Robert Morris, Jean-Sabin McEwen, Cathy Chin
- **9:06** Paper **461d:** Solvent Effects on CO Adsorption and Oxidation on Pt/Al₂O₃ Using FTIR-ATR Spectroscopy
- Wendi Guo, Ayman M. Karim
- **9:24** Paper 461e: Solvent Effects on Elementary Reactions in Solid-Acid Catalyzed Reactions: Acid-Base Interactions in Zeolites
- **Yanyu Mu**, William Elliott, Linxi Wang, Robert M. Rioux
- **9:54 Paper 461f:** Scaling Approaches to Solvent-Adsorbate Interactions

 Jaeryul Park, Luke Roling
- **10:12 Paper 461g:** Understanding the Promotional Role of Acids and Halides on Direct Synthesis of H₂O₂
- **Pranjali Priyadarshini**, David Flaherty

(462) Highly Selective Separations with Membranes I

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Barrel Spring I Dibakar Bhattacharyya, Co-Chair Stephen Ritchie, Co-Chair Christine Duval, Co-Chair

Sponsored by: Membrane-Based Separations

- **8:00** Paper 462a: Studies on the Potential of Graphene-Oxide Based Membranes for Waste Water Treatment *Mainak Majumder*
- **8:21** Paper 462b: Hydrophobic Thin-Film Composite Membranes Coated with UV-Curable Fluoropolymer for Concentrating Pharmaceuticals and Food Additives in Organic Solvents
- **Bofan Li**, Yue Cui, Neal Tai-Shung Chung
- **8:42 Paper 462c:** Novel Spirocyclic Polymers for Membrane-Based Organic Solvent Separations
- **Ronita Mathias**, Kirstie Thomspon, Dhaval Bhandari, JR Johnson, Huaxing Zhou, M.G. Finn, Ryan Lively

- **9:03 Paper 462d:** Membrane Separations with High Selectivity — *John Chau, Kamalesh K. Sirkar*
- **9:24** Paper 462e: Optimization-Based Computational Tools for Precise Engineering of Channel Proteins and Organic Cages to Perform Angstrom-Scale Separations
- Ratul Chowdhury
- 9:45 Paper 462f: Pi Electron Cloud Mediated Separation of Aromatics Using Supported Ionic Liquid (SIL) Membrane Having Antibacterial Activity
- Arijit Sengupta, Xianghong Qian, Ranil Wickramasinghe
- 10:06 Paper 462g: Continuous Zeolite MFI Membranes from 2D MFI Nanosheets on Ceramic Hollow Fibers: Fabrication Processes and Hydrocarbon Separation Properties
- **Byunghyun Min**, Shaowei Yang, Akshay Korde, Yeon Hye Kwon, Christopher W. Jones, Sankar Nair

(463) In Honor of Professor Rafiqul Gani's 65th Birthday (Invited Talks) Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 24

Venkat Venkatasubramanian, Chair Efstratios N. Pistikopoulos, Co-Chair

Sponsored by: Systems and Process Design

- **8:00 Paper 463a:** Rafiqul Gani Session: Introductory Remarks
- Venkat Venkatasubramanian
- **8:05** Paper **463b**: A Tribute to Professor Rafiqul Gani to Recognize His PSE Contributions over Many Years
- Warren D. Seider
- **8:25 Paper 463c:** Honoring Rafiqul Gani: Properties Are Central to PSE
- John P. O'Connell
- **8:45 Paper 463d:** Facing the Future of PSE: Challenges from Complex Real World Problems and Solutions
- Joan Cordiner
- **9:05** Paper **463e**: Design and Development of Innovative Chemical Products What's Next? *Ka Ng*
- **9:25 Paper 463f:** Next Generation Software Tools for Chemical Process and Product Design
- Mario Richard Eden
- **9:45** Paper **463g**: Development of MINLP Synthesizer Mipsyn-Global for Circular Synthesis of Sustainable Production Systems
- Zdravko Kravanja

10:05 Paper **463h:** Thermodynamic Analysis of the Driving Force Approach: Reactive and Non-Reactive Systems

- Eduardo S. Perez-Cisneros
- **10:25 Paper 463i:** Rafiqul Gani: Concluding Remarks
- Stratos Pistikopoulos

(464) In Honor of the 2019 Practice Award Winner (Invited Talks)

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Florida Ballroom B

Eranda Nikolla, Chair Jean-Sabin McEwen, Co-Chair Charles H. F. Peden, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 464a: Opening Remarks — *Eranda Nikolla*

8:10 Paper 464b: Impact of Water on Acid-Base Catalyzed Reactions

— Johannes A. Lercher

8:30 Paper 464c: Swellable

Organically Modified Silica (SOMS) As a Catalyst Scaffold for Catalytic Treatment of Water through Hydrogenation and Hydrogenolysis Reactions

— Umit S. Ozkan, Saurabh Ailawar, Anagha Hunoor, Gokhan Celik, Seval Gunduz, Jeffrey T. Miller, Franklin (Feng) Tao, Paul Edmiston

8:50 Paper **464d:** Mechanistic Studies of Direct Hydrodeoxygenation of *M*-Cresol over WOx-Decorated Pt Catalysts

— Cong Wang, Tianqi Chen, Raymond J. Gorte**, John Vohs**

9:10 Paper 464e: The Importance of Vapor Phase Transport during Accelerated Aging of Emission Control Catalysts

— Abhaya K. Datye

9:30 Paper 464f: Single Metal Atom Catalysts: A New Frontier in Heterogeneous Catalysis

— Sufeng Cao, Georgios Giannakakis, Mengyao Ouyang, Mengwei Li, **Maria Flytzani-Stephanopoulos**

9:50 Paper 464g: Alkene Dimerization on Grafted Ni Cations at Sub-Ambient Temperatures: Mechanism, Site Requirements, and Solvation Effects By Intrapore Liquids

— Iker Aguirrezabal Telleria, Shuai Wang**, Enrique Iglesia**

10:10 Paper 464h: Innovative Catalytic Materials of Industrial Relevance — *Yong Wang*

(465) Interfacial Aspects of Oil/Gas Recovery and Remediation

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom J Claribel Acevedo, Chair Joseph R. Samaniuk, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 465a: Characterizing Anionic surfactant Retention on Berea Sandstone

— **Reza Amirmoshiri**, Maura Puerto, Rouhi Farajzadeh, George J. Hirasaki, Sibani Lisa Biswal **8:15** Paper 465b: Demulsification of Non-Ionic Surfactant-Stabilized Emulsions from Enhanced Oil Recovery with Magnetic Nanoparticles

— **Leilei Zhang**, Zhuqing Zhang, Maura Puerto, George J. Hirasaki, Sibani Lisa Biswal

8:30 Paper 465c: A New Surfactant Evaluation Protocol Based on Interfacial Tension, Phase Behavior, and Lab-Scale Coreflood Tests for Chemical Enhanced Oil Recovery (cEOR) Applications

— **Jaeyub Chung**, Jeremy Holtsclaw, Thomas A. Everett, Timothy Henderson, Bryan W. Boudouris, Elias I. Franses

8:45 Paper **465d**: Effluent Analyses and Interfacial Tension Measurements for Laboratory-Scale Coreflood Oil Recovery Experiments

— **Jaeyub Chung**, Thomas A. Everett, Timothy Henderson, Jeremy Holtsclaw, Bryan W. Boudouris, Elias I. Franses

9:00 Paper 465e: Wettability Alteration of Carbonates By Mixed Anionic and Non-Ionic Surfactants

— **Soumik Das**, Quoc P. Nguyen, Roger T. Bonnecaze

9:15 Paper 465f: Adsorption of Lignin Nanoparticles at Oil-Water Interface: An Ecofriendly Approach to Oil Spill Cleanup

— **Jin Gyun Lee**, Luke L. Larive, Kalliat T. Valsaraj, Bhuvnesh Bharti

9:30 Paper **465g:** Probing Interfacial Structure and Dynamics of Asphaltenes and Model Asphaltenes at Fluid-Fluid Interfaces

— **J. Fernando Fajardo-Rojas**, Diego C. Pradilla, Oscar A. Alvarez, Joseph R. Samaniuk

9:45 Paper **465h**: Colloidal Stability and Interparticle Interactions of Proppant Dispersed in pH-Responsive, Supramolecular Hydraulic Fracturing Fluids

- Shuhao Liu, Mustafa Akbulut

10:00 Paper 465i: Adsorption and Remanence of Surfactants over Soil As Function of Mineralogy and Ionic Strength

— Tomás-Eduardo Chávez-Miyauchi, Adriana Benitez-Rico, Alejandro Islas-García

(466) Mammalian Synthetic Biology Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 3 Leonidas Bleris, Chair Nicholas R. Sandoval, Co-Chair Qing Sun, Co-Chair J. Andrew Jones, Co-Chair Piyush Jain, Co-Chair Peng Xu, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 466a: Design and Characterization of a Salicylic Acid-Inducible Gene Expression System for Mammalian Cells

— **Aarti Doshi**, Irfan Bandey, Dmitry Nevozhay, Navin Varadarajan, Patrick C. Cirino **8:18** Paper 466b: High-Pass Filtering and Noise Suppression in Intragenic miRNA-Mediated Host Regulation

— Taek Kang, Tyler Quarton, Kristina Ehrhardt, Chance M. Nowak, Abhyudai Singh, Yi Li, Leonidas Bleris

8:36 Paper 466c: Exploring and Exploiting Chromatin to Process Dynamic Optogenetic Signals — Jessica B. Lee, Jennifer Y. Lo, Nicholas Levering, Albert Keung

8:54 Paper 466d: Ultrasound Imaging of Gene Expression in Mammalian Cells
— Arash Farhadi, Gabrielle Ho, Daniel P. Sawyer, Raymond W. Bourdeau, Mikhail G. Shapiro

9:12 Paper 466e: Programmable Protein Circuits in Living Cells — *Xiaojing Gao*, *Lucy Chong, Matthew Kim, Michael Elowitz*

9:30 Paper 466f: EuGeneCD: A Computational Tool for Qualitative Genetic Circuit Design for Eukaryotic Organisms

— Wheaton Schroeder, Rajib Saha

9:48 Paper **466g**: Advancing the Frontiers of Design-Driven Engineering in Mammalian Synthetic Biology

- Joshua Leonard

(467) Medical Devices II Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration

Huanan Zhang, Chair Elizabeth Nance, Co-Chair

Sponsored by: Chemical Engineers in Medicine

8:00 Paper 467a: Highly Conductive, Stretchable, and Biocompatible Nanocomposite for Electromechanical Cardioplasty

- Dae-Hyeong Kim

8:21 Paper **467b**: Core-Shell Gallium/ Polymer Microstructure for Thermal-Responsive Implantable Electrode — *Taehwan Lim*, *Huanan Zhang*

8:42 Paper 467c: Morphing Electronics for Growing Tissue
— *Jinxing Li*

9:03 Paper **467d**: Soft and Biostable Silver - Gold Core - Shell Nanowire Nanocomposite Film — *Frank Curry Jr.*

9:24 Paper 467e: Nanowire Arrays Restore Vision in Blind Mice — *Jing Tang*

9:45 Paper 467f: Viscoelastic Aerosol: Novel Inhalation and Oro-Nasal Routes to Drug Delivery

— **Jerome Unidad**, Ravi Neelakantan, Jamie Kalb, Michael Benedict, David Johnson

(468) Membranes for Bioseparations Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Barrel Spring II Heather C. S. Chenette, Chair Stephen M. Ritchie, Co-Chair

Sponsored by: Bio Separations

8:00 Paper 468a: Factors Controlling Protein Transmission in Continuous Dynamic Filtration

— Henrik S. Marke, Martin P. Breil, Manuel Pinelo, Ernst Broberg Hansen, Ulrich Krühne

8:25 Paper **468b**: Understanding Membrane Fouling during a Combined Tangential-Flow and Depth Filtration Process

— **Ranil Wickramasinghe**, Da Zhang, Xianghong Qian, Daniel Strauss

8:50 Paper 468c: New Multimodal Anion-Exchange Membranes for Purification of Therapeutic Proteins

— Scott M. Husson, Joshua Osuofa, Daniel Henn, Anna Forsyth, Graham Temples, Jinxiang Zhou

9:15 Break

9:40 Paper 468e: A Membrane Process for the Purification of Nanosized Vesicles

— Eleonora Lalli, Gaia Gravili, Enrica Cortini, Thomas Fabiani, **Cristiana Boi**

10:05 Paper **468f**: Membrane Developments for Decellularization of Blood Via Gravity in Dry Plasma Spot Applications

— **Jie Gao**, Kwee Hiang Jackson Low, Chester L. Drum, E. Shyong Tai, Neal Tai-Shung Chung

(469) Microfluidic and Nanoscale Flows: Multiphase Systems and External Fields

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom M

Amanda B. Marciel, Co-Chair Sujit S. Datta, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 469a: Mixing By Asymmetrical Drop Coalescence in Microfluidics

- Mark Simmons

8:15 Paper 469b: Osmophoretic Motion of Semipermeable Polymersomes Driven By Solute Gradients in Microfluidic Channels — Yang Gu, Lisa Tran, Kyle J.M. Bishop

8:30 Paper 469c: Dynamics of Three Elastic Capsules in Square Microfluidic Channels

— **Pompon Mputu Udipabu**, Panagiotis Dimitrakopoulos

8:45 Break

9:00 Paper 469e: A Sheared Suspension of Conducting Particles in a Magnetic Field: Particle Rotation, Antisymmetric Stress and Secondary Flows

-Viswanathan Kumaran

9:15 Paper 469f: Controlling Immiscible Fluid Displacement Using Pore Size Gradients in Disordered Media — Nancy B. Lu, Christopher A. Browne, Daniel B. Amchin, Janine Nunes, Sujit S. Datta

- **9:30** Paper 469g: Continuous Synthesis of Organic/Inorganic Microparticles Using a Low-Cost Flow-Focusing Microreactor
- Milad Abolhasani
- **9:45** Paper 469h: Nonphotochemical Laser-Induced Nucleation of KCI Aqueous Solution in Microfluidics
- **Tianyi Hua**, Omar Gowayed, Danielle Grey-Stewart, Bruce A. Garetz, Ryan L. Hartman
- **10:00 Paper 469i:** Numerical Simulation of Microbubble Streaming: The Effect of the Bubble Protruded Depth on Flow Patterns
- **Behrouz Behdani**, Saman Monjezi, Jie Zhang, Cheng Wang, Joontaek Park
- **10:15 Paper 469j:** Dispersion and Mass Transfer of Microbubble in Capillary Embedded Step T-Junction Microchannel
- Yuchao Chen

(470) Mixing Scale-Up and Scale-Down Issues in Pharmaceutical and Biopharmaceutical Processes

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 32 Luis Sierra, Chair Matthew H. Flamm, Co-Chair Piero M. Armenante, Co-Chair

Sponsored by: North American Mixing Forum

- **8:00 Paper 470a:** Defining a Scale-up Strategy for an Oil in Water Cosmetic Emulsion
- Andrea Suaza, Alvaro Orjuela
- **8:21** Paper 470b: Effective Scale-up of Aerated Fermentation Processes with Complex Rheology to Industrial Scale *Sören Bernauer*, *Mathias Schöpf*, *Christian Witz*, *Philipp Eibl*, *Johannes G. Khinast*, *Timo Hardiman*
- **8:42** Paper **470c**: Direct Numerical Simulation of Bioreactors Using GPUs *John A. Thomas*
- **9:03 Paper 470d:** Using Numerical Modelling (CFD) to Expedite Scale-up and Technology Transfer of Industrial Bioprocesses between Manufacturing Sites
- Becca Dunne
- **9:24 Paper 470e:** Use of Acoustic Emission for Identifying Gas-Liquid Mixing Regime in Agitated Vessels at Different Scales Applying Machine Learning
- Giuseppe Forte, Federico Alberini, Mark Simmons, Hugh Stitt
- **9:45** Paper **470f**: Hydrodynamics Investigation of USP Dissolution Testing Apparatus I (Basket Apparatus) and Effect of the Basket Mesh Size on Hydrodynamic Characteristics
- **Chadakarn Sirasitthichoke**, Piero M. Armenante
- **10:06 Paper 470g:** Efficiently Characterize Process Scalability in the Micromixing-Mesomixing Space Using the Bourne Protocol
- Aaron Sarafinas

(471) Modeling and Design of Biopharmaceutical Processes

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 8 Nandkishor Nere, Chair Jacob Albrecht, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **8:00** Paper 471a: Development of a Segregated Cell Growth Model Structured By Dynamic Flux Balance Analysis
- **Rodrigo Barbosa**, Kirsty Skeene, Paloma Diaz-Fernandez, Gary Finka, Cleo Kontoravdi
- **8:21** Paper **471b**: A Holistic Modelling Framework Describing CHO Cell Metabolism and Both Antibody and Host Cell Protein Glycosylation
- **Pavlos Kotidis**, Ioscani J. del Val, Frederick Krambeck, Michael Betenbaugh, Cleo Kontoravdi
- **8:42** Paper **471c**: Dynamic Simulation and Process Assessment of Cultivation Modes in Monoclonal Antibody Production Using Pilot-Scale Experimental Data
- **Kozue Okamura**, Sara Badr, Hirokazu Sugiyama
- **9:03 Paper 471d:** Experimental Design, Error Modeling and Parameter Confidence in Chromatography
- **William Heymann III**, Pablo Rolandi, Eric von Lieres
- **9:24 Paper 471e:** Mathematical Modeling of the Freezing of Pharmaceutical Solutions
- Domenico Colucci, Davide Fissore, **Richard D. Braatz**
- **9:45** Paper 471f: Combining Numerical Modelling (CFD), Statistical Modelling (MVDA) and Laboratory Experiments for the Optimization of Large Scale UF/DF Operations
- Justin O'Sullivan, Damian Duffy
- **10:06** Paper **471g:** Engineering-Driven Application of Quality By Design to the Gmma Platform: Enabling the Production of Affordable and Effective Vaccines for Low and Middle Income Countries
- Maria M. Papathanasiou, Zoltán Kis, Luigi Sollai, Carlo Giannelli, Antonio Baccante, Anna Maria Colucci, Emilia Cappelletti, Ivan Pisoni, Elena Palmieri, Beatrice Ricchetti, Francesca Necchi, Oliver Koeberling, Laura B. Martin, Nilay Shah, Cristiana Campa, Francesca Micoli, Cleo Kontoravdi

(472) Nanomaterials for Light Harvesting and Novel Photophysical Phenomenon

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Discovery 46 Jinwoo Lee, Chair

Sponsored by: Nanomaterials for Energy Applications

8:00 Paper 472a: Efficient and Mechanically Robust All-Polymer Solar Cells

— Bumjoon J. Kim

- **8:35** Paper **472b**: Factors Governing Site Specific Rates of Electronic Excitations in Multicomponent Plasmonic Materials
- Steven Chavez, Suljo Linic
- **8:59 Paper 472c:** Advanced Li-Metal Batteries and Their Thermal Safety Aspects
- **Vilas G. Pol**, Patrick Kim, Dhanya Puthusseri
- **9:23 Paper 472d:** Quasi-2D Hybrid Organic-Inorganic Perovskites: DFT Modeling Approach
- Omar Allam, Ilgeum Lee, Dong Ha Kim, Seung Soon Jang
- **9:47** Paper **472e:** Carrier Dynamics of Photocatalytic Two-Dimensional Semiconductors Decorated with Plasmonic Nanoparticles
- **Jeremy R. Dunklin**, Aaron H. Rose, Hanyu Zhang, Jao van de Lagemaat
- **10:11 Paper 472f:** Development of Tandem Semiconductor Microparticles for Water-Splitting
- **Saumya Gulati**, Joshua Spurgeon

(473) Nanotechnology for Biotechnology and Pharmaceuticals

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Discovery 45 Nigel Reuel, Chair Aaron C. Anselmo, Co-Chair

Sponsored by: Bionanotechnology

8:00 Paper 473a: Synthetic-Biological Hybrid Nanoscale Systems for Drug Delivery

- Samir Mitragotri
- **8:31** Paper 473b: Engineering Muco-Inert Nanoparticles for Improved Vaginal Drug Delivery during Pregnancy
- **Hannah Zierden**, Jairo I. Ortiz, Kevin DeLong, Peter Dimitrion, Victoria Laney, Sabrine Bensouda, Justin Hanes, Laura Ensign
- **8:48** Paper 473c: Toward a Stable Single-Dose Oral Malaria Cure: Enhancing Dissolution Kinetics Using Continuous Nanoparticle Fabrication
- Kurt D. Ristroph, Jie Feng, Simon A. McManus, Yingyue Zhang, Kai Gong, Hanu Ramachandruni, Claire White, Robert K. Prud'homme
- **9:05** Paper 473d: Theranostic Nanocarriers Combining High Drug Loading, Heat Release, and Magnetic Particle Imaging
- Eric Fuller, Georg Scheutz, Angela Jimenez, Parker Lewis, Shehaab Savliwala, Sitong Liu, Brent S. Sumerlin, Carlos Rinaldi
- 9:22 Paper 473e: Translation of Nanoparticle Therapeutics from Laboratory Discovery to Clinical Scale: Scaled-up Production and Solidification Chang Tian, Jie Feng, Chester E. Markwalter, Leon Z. Wang, Madeleine Armstrong, Robert K. Prud'homme

- 9:39 Paper 473f: Engineering PLGA Nanoparticles to Encapsulate Large CRISPR-Cas_g Plasmids
- Ami Jo, Veronica Ringel-Scaia, Irving Allen, **Richey M. Davis**
- **9:56 Paper 473g:** Engineering Lipid Nanoparticles for Drug Delivery to Alleviate Oxidative Stress during Stem Cell Transplant Therapy
- **Rashi Porwal**, Stephen L. Hayward, Ou Wang, Yuguo Leo Lei, Srivatsan Kidambi

(474) New Methods and Developments in Computational Catalysis I

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom F Chris Paolucci, Chair Matthew Montemore, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00 Paper 474a:** Automated Generation of Metal-Doped Amorphous Silica Clusters
- Amy M. Jystad, Pubudu N. Wimalasiri, Ward H. Thompson, Marco Caricato
- **8:18** Paper **474b**: Amorphous Catalysts: Importance Learning Algorithm for Site Averaged Kinetics *Craig Vandervelden*, *Salman Khan, Susannah L. Scott, Baron Peters*
- **8:36 Paper 474c:** Rational Design of Alloy Catalysts
- **Tim Mueller**, Liang Cao
- **8:54** Paper **474d:** Bayesian Chemisorption Theory of Catalysis with Uncertainty Quantification
- **Siwen Wang**, Hongliang Xin
- 9:12 Paper 474e: Uncertainty
 Quantification of the Water-Gas Shift
 Reaction By Pt/CeO₂ Catalyst
 Eric Walker, Gabriel Terejanu, Salai
 C. Ammal, Andreas Heyden
- **9:30** Paper 474f: Improved Saddle Point Convergence with Dynamic and Selective Optimizations of Nudged Elastic Bands
- **Per Lindgren**, Georg Kastlunger, Andrew A. Peterson
- **9:48** Paper **474g**: Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis
- **Fang Liu**, Tzuhsiung Yang, Jing Yang, Eve Xu, Akash Bajaj, Heather J. Kulik

10:06 Paper **174ar:** Effectiveness Factor for Multi-Step Reactions — *M. Brennan Pecha*, Aaron Lattanzi, Vivek Bharadwaj, Peter N. Ciesielski (475) New Technologies to Enhance the Production of Unconventional Oil & Natural Gas: Experimentation & Simulation

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Challenger 40 Jared Ciferno, Chair Rameshwar D. Srivastava, Co-Chair Jason Trembly, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

8:00 Paper **475a**: Unconventional Oil and Natural Gas - Science & Technology Advancement

— Jared Ciferno

8:18 Paper 475b: The Potential for Enhanced OIL Recovery in the Bakken Petroleum System

— James A. Sorensen, Bethany Kurz, John A. Hamling, Steve Hawthorne, Charles D. Gorecki, John A. Harju, Edward N. Steadman

8:36 Paper 475c: Improved
Oil Recovery (IOR) Method for
Unconventional Reservoirs with a Next
Generation Huff-and-Puff Treatment
Combining Gas with Nanoparticles for
Enhancing Recovery

- Robin Watts

8:54 Paper **475d**: Gas Transport in Shale Matrix Coupling Multilayer Adsorption and Pore Confinement — *Di Chai*, *Zhaoqi Fan*, *Gang Yang*, *Xiaoli Li*

9:12 Paper 475e: Management of Iron Precipitation As a Solution for Decreased Petroleum Production from the Utica/ Point Pleasant Unconventional Play — Michael Spencer, Jason Trembly

9:30 Paper 475f: Reactive Transport in Shale Matrix after Fracturing Fluid Imbibition

— **Qingyun Li**, Adam D. Jew, Gordon Brown Jr., John Bargar, Kate Maher

9:48 Paper **475g**: Surfactant- or Nanoparticle-Stabilized CO₂-in-Oil and Natural Gas-in-Oil Emulsions and Foams for Completely Waterless Hydraulicfracturing

— Shehab Alzobaidi, Timothy Angeles, Gianfranco Rodriguez, Peter LeMaire III, Keith Johnston, **Robert Enick**

10:06 Paper **475**h: Boiling Points of Hydrocarbons in Nanoporous Media at High Pressures Using Differential Scanning Calorimetry Measurements — *Hyeyoung Cho*, *Taylor Jordan*, *Milind Deo*

(476) Novel Nanoparticles and Nanostructured Materials for Catalysis

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 19 J. Ruud van Ommen, Chair Yomaira Pagan-Torres, Co-Chair Kishori T. Deshpande, Co-Chair

Sponsored by: Nanoparticles

8:00 Paper 476a: Cerium Oxide Promoted Nickel Nanoparticles Deposited By Atomic Layer Deposition for Dry Reforming of Methane

— Baitang Jin, Zeyu Shang, Shiguang Li, Xinhua Liang

8:30 Paper 476b: The Impact of Support in Syngas Conversion over Rh-Mn Particles on WC

— **Florian Göltl**, Yifei Liu, Lifeng Zhang, James Dumesic, Manos Mavrikakis

8:48 Paper 476c: Modular Self-Assembly of Metal/Polymer Nanoreactors

— **Andrew Harrison**, Tien Vuong, Michael Zeevi, Benjamin Hittel, Christina Tana

9:06 Paper 476d: Gold Bimetallic Nanoparticles for Applications in Selective Oxidation Catalysis

— Joseph Brindle, Michael M. Nigra

9:24 Paper 476e: Role of Poly(*N*-vinylpyrrolidone) and Its Influence on Ag+ Reduction Kinetics during Formation of Ag Nanostructures

— Suprita Jharimune, Zhifeng Chen,

 Suprita Jharimune, Zhifeng Chen Justin Anderson, Ji Woong Chang, Robert M. Rioux

9:42 Paper **476f**: Enhancement of CO_2 Desorption Performances in CO_2 -Loaded MEA Solution By Using CMK-3 Bifunctional Catalysts

— **Zain Ali Saleh Bairq Sr.**, Zhiwu Liang, Hongxia Gao

10:00 Paper **476g**: Identification of Stable Bimetallic Nanoclusters Via a Mathematical Optimization Framework — *Xiangyu Yin*, *Natalie M. Isenberg*,

Xiangyu Yin, Natalie M. Isenberg,
 Michael G. Taylor, Giannis Mpourmpakis,
 Chrysanthos E. Gounaris

10:18 Paper **476h:** Oxidative Dehydrogenation of Ethane to Ethylene with Fe₂O₃@SiO₂ Core@Shell Catalysts — *Yahui Yang*, *Eyram Akabua*, *Götz Veser*

(477) Nucleation and Growth I Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Manatee Spring I

Meenesh R. Singh, Chair Marina Tsianou, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00 Welcoming Remarks

8:03 Paper 477a: Macromolecular Modulation of Calcium Oxalate Nucleation and Growth

— Gopichand Mallam, Arkita Chakrabarti, Junce Cheng, **Marina Tsianou**

8:24 Paper 477b: Direct Measurement of Growth Rate Dispersion in the Reactive Crystallization of Ampicillin Trihydrate

— **Matthew A. McDonald**, Andreas S. Bommarius, Martha A. Grover, Ronald W. Rousseau

8:45 Paper **477c:** Dynamics of Struvite Formation: Insights from the Macroscopic to Molecular Scale

— Doyoung Kim, Chara Olympiou, Nicola Irwin, Jeffrey D. Rimer

9:06 Paper 477d: Comparative Screening of Polymorphs of o-Aminobenzoic Acid Using Microtiter Plates and Novel Continuous-Flow, Microfluidic Devices

— **Paria Coliaie**, Manish S. Kelkar, Nandkishor Nere, Meenesh R. Singh

9:27 Break

9:48 Paper 477f: Environmentally Friendly Molecular Modifiers Reveal Unique Inhibition and Dissolution Mechanisms in Barite Scale

— **Ricardo D. Sosa**, Xi Geng, Jeremy C. Palmer, Michael A. Reynolds, Jacinta C. Conrad, Jeffrey D. Rimer

10:09 Paper **477g**: Nucleation Behavior of Ethyl Vanillin: The Partial Dependence of Kinetic Parameters on Interfacial Energy

— **Jing Yang**, Shijie Xu, Jingkang Wang, Junbo Gong

(478) Panel on Pre-Competitive Collaboration (Invited Talks) Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 6 Jean W. Tom, Chair

Andreas S. Bommarius, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Introductory Remarks

8:05 Paper 478a: IQ Consortia and Pre-Competitive Information Exchange — *Kevin D. Seibert, Timothy Curran, John F. Traverse*

8:23 Paper 478b: Lhasa Limited-Achieving Innovation through Collaborative Progress

— Liz Covey-Crump, Crina Heghes,

David Yeo 8:41 Paper 478c: NIIMBL -the National Institute for Innovation in Manufacturing

Biopharmaceuticals

— Kelvin H. Lee

8:59 Paper 478d: Sage Bio Networks-Searching for Mutual Incentives: The Sweet Spot for Collaboration — *Brian Bot*

9:17 Paper 478e: Enabling Technologies Consortium: A New Paradigm for Pre-Competitive Collaboration on Technology — Jean Tom, Aaron Cote, James M.

Vergis
9:35 Paper 478f: FDA's Emerging
Technology Program: Innovation and

Collaboration to Advance Product Quality
— *Thomas O'Connor*, Sau Lee, Cecilia
Cruz

9:53 Panel Discussion

(479) Particulate and Multiphase Flows: Colloids and Grains Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom L Javen Weston, Co-Chair Christopher L. Wirth, Co-Chair Charles E. Sing, Co-Chair Ya-Wen Chang, Co-Chair

Sponsored by: Fluid Mechanics

8:00 Paper 479a: Cracking and Self-Healing of Shrinkable Granular Packings — *H. Jeremy Cho, Sujit S. Datta*

8:15 Paper 479b: Fiber Alignment in Confined Shearing Flows
— Scott Strednak, Laurence
Bergougnoux, Elisabeth Guazzelli,
Jason E. Butler

8:30 Paper **479**c: Head-on and Oblique Collisions of Wet Particles — *Robert Davis*, *Jake Sitison, Riley Shore*

8:45 Paper **479d**: The Effect of Rpm and Particle Number on the Solid-Liquid Mixing Tank Performance: Application of CFD-DEM and ERT Experimental Measurements

— **Mohammadreza Ebrahimi**, Richard Wood, Argang Kazemzadeh, Farhad Ein-Mozaffari

9:00 Paper 479e: Effects of Particle Shape on Shear-Induced Aggregation/ Fragmentation and Viscosity of Boehmite Crystal Suspensions — Jaehun Chun, Anthony Krzysko, Lawrence Anovitz, Cornelius F. Ivory, Jan llovsky, Ivan Kuzmenco, Gregory Schenter, Sue Clark

9:15 Paper 479f: Microstructure and Rheological Properties of Oil-Based Drilling Fluids

— **Manizheh Ansari**, Dinesh V. Kalaga, Damon Turney, Jeffrey F. Morris, Sanjoy Banerjee, Masahiro Kawaji

9:30 Paper **479g**: A Non-Local Constitutive Model for Dense Granular Flows That Incorporates Shear-Induced Dilation

— Prabhu R Nott

9:45 Paper 479h: The Transition from Steady Non-Oscillatory Flow to Oscillatory Flow of Granular Material through a Vertical Channel: A DEM Study — Bhanjan Debnath, Viswanathan Kumaran, Kesava Rao Kaza

10:00 Paper **479i**: Forces on Non-Spherical Particle in the Vicinity of Rough Wall at Finite Reynolds Number — *Atul M. Bhagat, Partha S. Goswami*

10:15 Paper 479j: Turbulence Collapse in a Dilute Particle-Gas Suspension —Viswanathan Kumaran, Ankit Tyagi, Pradeep Muramalla, Partha S. Goswami

(480) Properties and Phase Equilibria for Fuels and Petrochemicals I

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Challenger 38/39

Paul M. Mathias, Chair M. R. Riazi, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 480a: Prediction of the Fugacity of Hydrogen Gas Dissolved in Organic Solvents with Emphasis on the High-Temperature High-Pressure Subcooled Liquid State

- Eric L. Cheluget

- **8:25** Paper **480b**: Pseudo-Component Techniques for Prediction of Thermophysical Properties of Hydrocarbon Mixtures and Fuels up to High Temperatures and Pressures
- Houman Rokni**, Joshua D. Moore**, Ashutosh Gupta, Mark A. McHugh, Manolis Gavaises
- **8:50 Paper 480c:** Development of a Thermodynamic Model and Multiphase Equilibrium Flash for Prediction of Crystallization in LNG Processes
- **Nevin Gerek Ince**, Freddy Garcia, Jean-Jacques Bartuel, Michael S. Kirchner, Seiya Hirohama, David Bluck
- **9:15 Paper 480d:** Advances in Modeling Asphaltene Precipitation and Deposition
- **Francisco Vargas**, Caleb Sisco, M.-R. Riazi
- **9:40 Paper 480e:** A Study of Unexpected Autoignition Temperature Trends for Pure N-Alkanes
- **Mark E. Redd**, Thomas A. Knotts IV, Neil Giles, W. Vincent Wilding

10:05 Paper **480f**: Investigation of the Flammability Limits of Petroleum Liquids — *Paul M. Mathias*

(481) Reaction Engineering in Pharmaceuticals and Fine Chemicals

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom E Anuj A. Verma, Chair Gaurav Giri, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper **481a**: Designing a Continuous Flow System to Safely Nitrate Alkylamines to Nena's *Jerry S. Salan, Trevor M. Rosensohn,*
- Jerry S. Salan, Trevor M. Rosensof Andrew G. Pearsall, Matthew L.
 Jorgensen, David J. am Ende
- 8:15 Paper 481b: Continuous
 Enzymatic Production of Enantiopure
 Amines in a Packed Bed Recycle Reactor
 Robert D. Franklin, Adam A.
 Caparco, Joshua A. Whitley, Bettina
 Bommarius, Julie A. Champion, Andreas
 S. Bommarius
- **8:30 Paper 481c:** 3D Printed Fixed Bed Catalytic Monolith for Continuous Chemistry
- **Brian R. Clark**, Sarah Smith, Frank Gupton, James K. Ferri

- 8:45 Paper 481d: Surface Plasmon Resonance Spectroscopy As a Tool for Distinguishing Homogeneous Versus Heterogeneous Catalytic Pathways for Metal Nano-Catalyzed C-C Coupling Reactions
- **Farshid Mohammadparast**, Marimuthu Andiappan
- **9:00** Paper 481e: Integrated Thermodynamic and Mechanistic Model of Homogeneous Catalytic *N*-Oxidation Processes
- **Jingyao Wang**, M. Sam Mannan, Benjamin A Wilhite
- **9:15 Paper 481f:** Impinging Jet for a Flow Synthesis of Mixing Sensitive Pharmaceutical Molecule
- **Anuj A. Verma**, Shashank Shekhar, Kushal Sinha, Moiz Diwan
- **9:30 Paper 481g:** Challenges and Successes in Continuous Chemical Processing
- **Andrew G. Pearsall**, Jerry S. Salan, David J. am Ende
- **9:45** Paper 481h: Chemical Processes Optimization By Hydrodynamic Simulations Implementation in the Solid Phase Peptide Synthesis
- Moshe Bentolila
- **10:00** Paper **481i:** Modelling, Design and Operation of a Continuous Cryogenic Reaction
- Christos Panos, **Flavien Susanne**, Neil Curtis, Markus Andersson, Sean Sisk

(482) Recent Advances in Molecular Simulation Methods II

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Rock Spring I/II Andrew White, Chair Harish Vashisth, Co-Chair Jindal K. Shah, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

- **8:00** Paper **482a**: Partial Molar Properties from Molecular Simulation Using Multiple Linear Regression
- Tyler R. Josephson, J. Ilja Siepmann
- **8:15 Paper 482b:** Improvements of the Continuous Fractional Component Monte Carlo Method
- **Ahmadreza Rahbari**, Remco Hens, Thijs J. H. Vlugt
- **8:30 Paper 482c:** Improving the Efficiency of Monte Carlo Simulations of Charged Molecules in the Grand Canonical Ensemble
- **Harold W. Hatch**, Steven Hall, Jeffrey Errington, Vincent K. Shen
- **8:45 Paper 482d:** Mapped-Averaging Formulations for Evaluation of Singlet and Multibody Density Distributions
- **Apoorva Purohit**, Andrew J. Schultz, Andrij Trokhymchuk, David A. Kofke

- **9:00 Paper 482e:** Filling Molecular Enclosures Using a Spliced Soft-Core Potential with Simulated Annealing Algorithm Development and Application to Ionic Liquids
- Austen Bernardi, Eric Meshot, Roland Faller
- 9:15 Break
- 9:30 Paper 482f: Azide and Alkyne Charmm Parameterization: Resolving Dihedral Interactions That Contain Linear Moieties
- **Addison K. Smith**, Thomas A. Knotts IV
- **9:45** Paper **482g**: Large-Scale Free-Energy Calculations in Metal-Organic Framework Prototypes
- **Ryther Anderson**, Diego Gomez Gualdron
- **10:00 Paper 482h:** Designing Anion Exchange Membranes with Improved Ion Conductivity By Mesoscale Simulations
- Ming-Tsung Lee

10:15 Paper **482i**: Ultrafast Detonation of Hydrazoic Acid:Insights from Many-Body Moleculardynamics Force Fields — *Cong Huy Pham, Nir Goldman, Laurence F. Fried*

(483) Scale-up, Revamp, and Industrial Applications of Adsorption

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Regency Ballroom U Robert Giraud, Chair

Roger D. Whitley, Co-Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper **483a**: Scaling up PSA for Renewable Energy Applications

— Kent Knaebel Jr.

8:30 Paper 483b: 23 Years of Adsorption and Ion Exchange: Lessons Learned

- Stephen Breske

9:00 Paper 483c: Accurately Modeling Liquid Phase Adsorption for Industrial Applications with Bench Scale Testing — *Christie Theys*

9:30 Paper 483d: Development of Adsorption Processes for the Separation of Close-Boiling Gas Mixtures

— **Abdulmalik Ajenifuja**, Lisa Joss, Megan Jobson

10:00 Paper **483e:** Advancements in Scaling up Metal Organic Framework (MOFs) Materials

 Jose Arno, Patrick Fuller, John Siegfried, Roberto Flores, William Morris, Omar Farha

(484) Sensor Development Platforms Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 10 Gozde Sultan Demirer, Chair Evan K. Wujcik, Co-Chair Xiao-an Fu, Co-Chair

Sponsored by: Sensors

- 8:00 Paper 484a: Photoelectrochemical Sensor — *Jing Tang*
- 8:15 Break
- **8:30** Paper **484c:** High-Throughput Sensing of Single-Bacterium Growth: Toward Rapid Antibiotic Susceptibility Testina
- Donghui Song, Haomin Liu, Huayi Ji**, Yu Lei**
- **8:45** Paper 484d: Ionophore-Based Optical Sensors Incorporating Long-Lifetime Phosphorescent Microparticles for Background-Free Ion Detection in Biological Samples
- **Mark S. Ferris**, Madeline Behr, Kevin J. Cash
- **9:00 Paper 484e:** Nanoplasmonic Quantification of Pathogen-Derived Extracellular Vesicles in Plasma Microsamples
- Tonv Hu
- **9:15 Paper 484f:** Quantification of Biomarkers at Point of Need Using Metal Enhanced Fluorescence and Surface Acoustic Waves
- Shuangming Li, **Yuqi Huang**, Venkat R. Bhethanabotla
- **9:30** Paper **484g**: High-Throughput Scanning Electrochemical Microscopy Based on Nonlocal Continuous Line Probes
- **Anna Dorfi**, Han-Wen Kuo, John Wright, Daniel Esposito
- **9:45** Paper **484h**: Solvent-Resistant Electrochemical Transistors As Dual Sensing Platforms in Aqueous and Organic Media
- **Brian Khau**, Lisa Savagian, James Ponder, Michel De Keersmaecker, John Reynolds, Elsa Reichmanis

10:00 Paper **484i**: Investigation of Polymer-Plasticizer Blends for BTEX Sensing Using Acoustic Wave Devices — *Abhijeet Iyer*, *Deekshitha*

— Abhyeet Iyer, Deekshitha Adapa, Scott W. Campbell, Venkat R. Bhethanabotla 10:15 Paper 484j: Microfabricated

Silion Nanowire Array Platform for Surface Enhanced Raman Spectroscopy — Jack T Lockard, Zhenzhen Xie, Xiao-an Fu

(485) Soft Matter Electrokinetics Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Plaza

International Ballroom I
Ning Wu, Chair
Christopher L. Wirth, Co-Chair

Sponsored by: Interfacial Phenomena

8:00 Paper 485a: Encoding Biomimetic 3D Helical Motion in Active Particles Using Induced-Charge Electrophoresis

— **Jin Gyun Lee**, Allan M. Brooks, William A. Shelton Jr., Kyle J.M. Bishop, Bhuvnesh Bharti

- **8:15 Paper 485b:** Electro-Hydrodynamic Extraction of Nucleic Acids from Bovine Serum
- **Benjamin Valley**, Anne D. Crowell, Jason E. Butler, Anthony J.C. Ladd
- **8:30** Paper **485**c: Geometrically Patterned Interfaces on Neat and Composite Polymeric Films By Electrohydrodynamic Film Patterning *Elif Karatay*, *Eric Weflen*, *Michael Benedict*, *David Johnson*
- **8:45** Paper **485d**: Diffusiophoretic Velocity for Mixture of Electrolytes with Asymmetric Ion Valences
- **Ankur Gupta**, Bhargav Rallabandi, Jessica Wilson, Suin Shim, Howard A. Stone
- 9:00 Paper 485e: Electrohydrodynamic Flow Around a Colloidal Sphere Under AC Electric Fields: A Combined Theoretical and Experimental Study
- Xingfu Yang, Ning Wu
- **9:15 Paper 485f:** Influence of Interfacial Forces on the Propulsion of Active Colloids
- Marola W. Issa, Nicky R. Baumgartner, Shawn D. Ryan, **Christopher L. Wirth**
- **9:30** Paper **485g**: Electrokinetic Enhancement of Ion Transport in Microfluidic Desalination Systems *Anne Benneker*
- **9:45** Paper **485h**: Opposing Trends in Surface Water Mobility for Ordered Mesoporous Silicas As a Function of Surface Polarity
- **Hyunjin Moon**, Song-I Han, Susannah L. Scott
- 10:00 Paper 485i: 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, Michael Strano

(486) Stem Cells and Tissue Engineering

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 1 Umut Gurkan, Co-Chair Amir M. Farnoud, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **8:00 Paper 486a:** Deriving Cerebellum-like Organoids from Induced Pluripotent Stem Cells
- **Thien Hua**, Julie Bejoy, Liqing Song, Yan Li, Qing-Xiang Amy Sang
- **8:18 Paper 486b:** The Assembly of Novel Human 3D Liver Tissues Using Induced Pluripotent Stem Cells
- **Lauren Wills**, Padmavathy Rajagopalan
- **8:36 Paper 486c:** Deep Profiling of Heterochromatin Associated Proteins and Their Role in Liver Cell Reprogramming
- **Bomyi Lim**, Samuel Keller

- **8:54** Paper 486d: Engineered Microenvironment for Manufacturing Human Pluripotent Stem Cell-Derived Vascular Smooth Muscle Cells
- **Ou Wang**, Haishuang Lin, Qian Du, Qiang Li, Chi Zhang, Yuguo Leo Lei
- **9:12** Paper **486e**: Production of Cardiac Tissue Spheroids from Encapsulated Hipscs Using a Novel Microfluidic System
- Ferdous Finklea, Petra Kerscher, Wen J. Seeto, Yuan Tian, **Elizabeth Lipke**
- **9:30 Paper 486f:** Restoration of Cellular Homeostasis of Human Mesenchymal Stem Cells during in Vitro Culture Expansion
- **Xuegang Yuan**, Yijun Liu, Brent Bijonowski, Qin Fu, Teng Ma
- **9:48 Paper 486g:** Invited: Bioengineering of Pancreatic Islet Organoids from Hpscs
- Ipsita Banerjee

(487) Sustainable Engineering Forum Plenary (Invited Talks)

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Regency Ballroom T Ignasi Palou-Rivera, Chair Fengqi You, Co-Chair

Sponsored by: Sustainable Engineering Forum

- **8:00 Paper 487a:** Sustainable Development for the Chemical Industry Through Process Intensification
- David R. Shonnard
- **8:45** Paper **487b**: Education for Enabling Sustainable Development: Role of Chemical Engineering and of the Campus as a Living Laboratory
- Bhavik R. Bakshi
- **9:30 Paper 487c:** Data-Driven Optimization for Sustainable Energy Systems
- Chao Ning, Fengqi You

(488) Sustainable Fuel from Renewable Resources

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Rainbow Spring I/II

Hyun-Tae Hwang, Chair Gerardo J. Ruiz-Mercado, Co-Chair

Sponsored by: Sustainability

- **8:00 Paper 488a:** Two-Step Sub/ Supercritical Water and Ethanol Processes for Non- Catalytic Biodiesel Production
- **ASO Hassan**, Hayder Alhameedi, Joseph D. Smith
- **8:20 Paper 488b:** Advances in Ultrasound- and Cavitation-Assisted Catalyzed Conversions of Biomass to Biofuels
- Yusuf G. Adewuyi

- **8:40 Paper 488c:** Biogasification of Cellulosic Ethanol Stillage in an Anaerobic Fluidized Bed Bioreactor
- Shunchang Yang, Clement
 Tseng, Gayathri Ram Mohan, Na
 Wu, Lonnie Ingram, Keelnatham
 Shanmugam, Spyros Svoronos, Pratap
 Pullammanappallil
- **9:00 Paper 488d:** Solar Powered Pyrolysis of Biomass with Catalytic Oxygen Carrier Regeneration
- **Asif Hasan Rony**, Maohong Fan
- **9:20** Paper **488e**: Biomass Utilisation Network Life-Cycle Optimisation for the Satisfaction of Energy, Fuels and Chemicals in the European Union
- **Raul Calvo-Serrano**, Carlos Pozo Fernández, Ángel Galán Martín, Miao Guo, Gonzalo Guillén-Gosálbez
- 9:40 Paper 488f: Comparative Economic and Environmental Assessments of Methanol Production from CO₂: Transport Vs. Energy
 Amjad Al-Qahtani, Andres Gonzalez, Carlos Pozo Fernández, Ángel Galán Martín, Gonzalo Guillén-Gosálbez

(489) Theory, Modeling, and Simulation of Nuclear Chemical Processes I

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Discovery 43 Maximilian B. Gorensek, Chair Valmor F. de Almeida, Co-Chair

Sponsored by: Nuclear Engineering Division

- **8:00** Paper **489**a: Habit 2.1: Assessing Consequences of Chemical Releases on Control Room Habitability Considering the Impact of a Dividing Streamline
- **Thomas O. Spicer III**, Casper Sun, Syed I. Haider
- **8:22 Paper 489b:** Natural Circulation in a VERY High Temperature Reactor (VHTR)
- **Dinesh V. Kalaga**, Apoorva Rudra, Masahiro Kawaji
- **8:44** Paper **489c:** Speciation of Fuel and Fission Products in Molten Salt Solutions from Ab Initio Molecular Dynamics
- Austin Clark, Stella D. Nickerson
- **9:06 Paper 489d:** Density Functional Theory Study of the Tritium Diffusion, Desorption, and Trapping on the γ-LiAlO₂ (100) Surface
- Ting Jia, David J. Senor, Yuhua Duan
- **9:28** Paper **489e**: Fundamental Studies of Tritium Diffusivity in Carbon Doped Defective γ-LiAIO, Pellets
- **Hari Paudel**, Yuhua Duan, David J. Senor
- **9:50** Paper **489f**: Modeling of Pluggage and Spatial Distribution of Particulate Matter Deposited in the Savannah River Site H-Canyon Process Vessel Vent Filters
- **James E. Laurinat**, Michael G. Bronikowski

- **10:12** Paper **489g**: Solvent Extraction Flowsheet-Level Modeling and Simulation with Radiolysis

 Valmor F. de Almeida, Kevin Ivon
- **Valmor F. de Almeida**, Kevin Lyon, Taha Azzaoui

(490) Thermophysical Properties: Complex Systems

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Silver Spring

Erik E. Santiso, Chair Clare McCabe, Co-Chair Sanket A. Deshmukh, Co-Chair Hiroyuki Matsuda, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **8:00** Paper 490a: Global Phase Diagrams of Binary and Ternary Mixtures of CH₄, CO₂, and H₂S: Experimental Measurements and Modeling
- Measurements and Modeling

 Marco Campestrini, Stefano Langé,
 Paolo Stringari, Laura Pellegrini
- **8:16** Paper 490b: Thermodynamic Properties and Molecular Interactions of Azeotropic Mixtures Using Molecular Simulation and Modeling
- **Dongyang Li**, Naveen Kumar Vasudevan, Xingang Li, Hong Li, Xin Gao, Li Xi
- **8:32** Paper 490c: Statistical Mechanics of Crystallization and Vitrification

 Muhammad R. Hasyim, Kranthi K. Mandadapu
- **8:48** Paper **490d**: Coarse-Grained Force Field for Asphaltene Model Compounds: Application to the Prediction of Their Thermodynamic Properties
- Caroline Desgranges, **Jerome Delhommelle**
- **9:04** Paper **490e**: Predicting Phase Equilibria and Thermodynamic Properties Using *Ab* Initio Potentials *Richard J. Sadus*
- **9:20 Paper 490f:** A Composite-Sphere Model for Janus Colloids with Central Force Potentials: Structures, Thermodynamic Properties, and Phase Behavior
- Lloyd L. Lee
- **9:36 Paper 490g:** Solubility of Carbon Dioxide in the Ionic Liquid Alkyl-3-Methylimidazolium Tricyanomethanide ([Cnmim]-[TCM]) Using a Magnetic Suspension Balance
- Muhammad Khan, **Cornelis Peters**, Sabbir Samdani
- **9:52 Paper 490h:** A Classical Density-Functional Theory Study of the Body-Centered-Cubic and Cl₁₆ Solid Phases of Hard Spheres
- **David M. Ford**, Vadim B. Warshavsky, Peter A. Monson
- **10:08 Paper 490i:** Co-Oriented Fluid Functional Equation for Electrostatic Interactions
 - Kai Langenbach

(491) Transport Phenomena, Rheology, and Mixing in Food **Processing and Engineering (Invited** Talks)

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 9 De-Wei Yin, Chair

Sponsored by: Food Innovation and Engineering

8:00 Paper 491a: Design of Mixing **Equipment for Rheologically Complex** Fluids

— Richard K. Grenville

8:25 Paper 491b: Invited Talk No. 3 in Transport Phenomena, Rheology, and Mixing in Food Processing and Engineering

- Christopher Tyler

8:50 Paper 491c: Invited Talk No. 2 in Transport Phenomena, Rheology, and Mixing in Food Processing and Engineering

9:15 Paper 491d: Invited Talk No. 4 in Transport Phenomena, Rheology, and Mixing in Food Processing and Engineering

9:40 Paper 491e: Invited Talk No. 5 in Transport Phenomena, Rheology, and Mixing in Food Processing and Engineering

10:05 Paper 491f: Invited Talk No. 6 in Transport Phenomena, Rheology, and Mixing in Food Processing and Engineering

(492) Understanding Powder **Processing via Materials Science**

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Celebration 14 Anil Rane, Chair Parind Desai, Co-Chair Pavithra Sundararajan, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and **Manufacturing Forum**

8:00 Paper 492a: Packing Prediction of Pharmaceutical Powders Via Bond **Number Estimation**

— Kuriakose Kunnath, Rajesh Davé

8:21 Paper 492b: Theoretical and Experimental Investigation into the Impact of Tribo-Charging on the Performance of Dry Powder Blends

– Joana T. Pinto, Sarah Zellnitz, Michael Brunsteiner, Thomas Wutscher, Amrit Paudel

8:42 Paper 492c: Influence of an External Lubricant on the Tribo-Charging Behaviour of Capsules

- Thomas Wutscher, Sarah Zellnitz, Mirjam Kobler, Francesca Buttini, Laura Andrade Benítez, Verónica Daza Fernández, Alberto Mercandelli, Stefano Biserni, Susana Ecenarro Probst, Amrit Paudel

9:03 Paper 492d: Investigation into the Effects of Roller Compaction on Granule and API Properties

- James Clarke, John Gamble, John Jones, Mike Tobyn, Richard Greenwood, Andrew Ingram

9:24 Paper 492e: In-Depth **Experimental Analysis of Pharmaceutical** Continuous Twin-Screw Wet Granulation in View of the Development of a Generic Compartmental PBM

- Michiel Peeters, Daan Van Hauwermeiren, Alexander Ryckaert, Christoph Portier, Tamas Vigh, Ashish Kumar, Fanny Stauffer, Jonathan Meyer, Jérôme Mantanus, Pankaj Doshi, Kai Lee, Ingmar Nopens, Thomas De Beer

9:45 Paper 492f: The Use of T-PLS to Investigate the IMPACT of Raw Material Properties on Granule Quality Attributes Obtained after Continuous Twin-SCREW WET Granulation

— Alexander Ryckaert, Jens Dhondt, Thomas De Beer

10:06 Paper 492g: Visualization of Granule Temperature Along the Length of the Barrel Using Thermal Imaging to Improve Process Understanding of Pharmaceutical Twin-Screw Melt Granulation

- Shana Van de Steene, Chris Vervaet, Thomas De Beer

(493) Young Faculty Forum (Invited Talks)

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Bayhill 29/30 Michael M. Nigra, Chair Jennifer Weiser, Co-Chair

Sponsored by: Young Faculty Forum

8:00 Paper 493a: Remaining True to Yourself

- Marc-Olivier Coppens

8:30 Paper 493b: Reflections from Ten Years at the Lectern: Insights on Teaching, Scholarship, and Service from an Educational-Focused Perspective

- Daniel Lepek

9:00 Young faculty networking

(494) Ammonia Safety Wednesday, Nov 13, 10:20 AM

Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

10:20 Paper 494a: Safety of Ammonia As Hydrogen and Energy Carriers

- Yoshitsugu Kojima

10:38 Paper 494b: Safe and Effective Application of Ammonia As a Marine Fuel

- Niels de Vries

10:56 Paper 494c: Ammonia Safety Placeholder Talk

- Trevor Brown

(495) John M. Prausnitz AIChE **Institute Lecture**

Wednesday, Nov 13, 11:15 AM Hyatt Regency Orlando, Plaza International Ballroom H Venkat R. Bhethanabotla, Chair

Sponsored by: Awards Committee

11:15 Paper 495a: From Chemical Engineering Fundamentals to the Commercialization of Vapor Deposited **Polymers**

- Karen K. Gleason

(496) 3D Printing in Pharmaceutical and Health Industry

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 28 Nima Yazdanpanah, Chair Yash Kapoor, Co-Chair

Sponsored by: 3D Printing

12:30 Paper 496a: 3D Printing: A New Era of Precise Manufacturing of Individually Developed Pharmaceuticals – **Ahmed Zidan**, Alaadin Alayoubi, Sarah Asfari, Nima Yazdanpanah, Thomas O'Connor, Muhammad Ashraf, Celia N. Cruz

1:05 Paper 496b: Smart Design and Virtual Product Analysis for 3D Printing Pharmaceutical Tablets for Patient Centric Product Development

- Nima Yazdanpanah, Ahmed Zidan, Alaadin Alayoubi, Sarah Asfari, Muhammad Ashraf, Celia N. Cruz, Thomas O'Connor

1:24 Paper 496c: Rapid on-Site Manufacturing Approach with 3DP Capsules: Delayed Burst Release for Regional Absorption

- Derrick Smith, Yash Kapoor, Gerard Klinzing, Andre Hermans, Rebecca Nofsinger, Kimberly Manser, Rebecca Nissley, Jessica Schlegel, Adam Procopio

1:43 Paper 496d: Production of Small-Batches of 3D Printed Multi-Compartment Capsular Devices for Oral Drug Delivery Using High-Throughput Robotic Manufacturing Technologies Alice Melocchi, Federico Parietti

2:02 Paper 496e: Pharmaceutical Application of Inkjet Based 3D Printing Process

Koyel Sen, Sameera Sansare, Si W. Li. Bodhisattwa Chaudhuri. Anson Ma

2:21 Paper 496f: 3D Printed Tablets Using Binder Jetting and Pharmaceutical Excipients

- Anthony Antic, Jun Zhang, Negin Amini, David Morton, Karen Hapgood

2:40 Paper 496g: Potential of 3D **Printing in Precision Combination** Therapy: A Case Study of Cardiovascular

Alaadin Alayoubi, Sarah Asfari, Michael Kopcha, Muhammad Ashraf, Celia N. Cruz, Ahmed Zidan

(497) Advances in Algal Biorefineries Wednesday, Nov 13, 12:30 PM

Hyatt Regency Orlando, Regency Ballroom V

Sridhar Viamajala, Chair Robert Gardner, Co-Chair Lynn Wendt, Co-Chair

Sponsored by: Sustainable **Biorefineries**

12:30 Paper 497a: Integrating Direct Air Carbon Capture and Algal-Based **Bioenergy Production**

- Maria Camila Caceres Falla, Hector De la Hoz Siegler Jr.

12:55 Paper 497b: Effects of Impurities in Two-Step Vs. One-Step Hydroprocessing of Algae Oils - Jacob S. Kruger, Earl Christensen, Tao Dong, Gina Fioroni, Nicholas J. Nagle, Philip Pienkos, Robert

1:20 Paper 497c: Integrated Microalgal Biorefinery: Optimization of Process Conditions for Enhanced Biofuel and Antioxidant Production

— **Safina Ujan**, Hector De la Hoz Siegler Jr.

McCormick

1:45 Paper 497d: Synthesis of Value Chains Towards Flexible Algae **Biorefineries Under Uncertainty** Melina Psycha, Antonis C. Kokossis

2:10 Paper 497e: Evaluating the Effectiveness of Plantain Peel Ash Extract As Bio-Based Alkali for Inducing

Flocculation of Microalgae - Sheriff Ajala, Matthew L. Alexander

(498) Advances in Bioprocess Design for Cell Culture and Bioproduct **Production**

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 4 Clayton Jeffryes, Co-Chair Aravindan Rajendran, Co-Chair Amit Kumar Jha, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 498a: MODEL-Free Simulation and Fed-Batch Control of Cyanobacterial Phycocyanin Production By Artificial Neural Network and DEEP Reinforcement Learning

— Yan Ma, Michael G. Benton, Jose A. Romaanoli

12:48 Paper 498b: Manufacturing **Process Development of Gesicles** - Juliette Champeil, Mathias Mangion, Rénald Gilbert, Bruno Gaillet

1:06 Paper 498c: Measures and Models for Production of Zika Virus Vaccines

- Huicheng Shi, John Yin

1:24 Paper 498d: Zinc Supplementation Improves the Harvest Purity of β-Glucuronidase in CHO Cell Culture By Suppressing Apoptosis

- Ryan Graham, Stephanie Ketcham, Adil Mohammad, Seongkyu Yoon, Chikkathur N. Madhavarao

- 1:42 Paper 498e: Simplified Lab Scale and Pilot Scale Bioreactor Processes for Recombinant Butyrylcholinesterase Production in Transgenic Rice Cell Suspension Cultures
- **Kantharakorn Macharoen**, Min Du, Karen A. McDonald, Somen Nandi
- 2:00 Paper 498f: Design and Manufacture of Novel Airlift Milibioreactors: A Low-Cost Lab Scale Approach for Proof-of-Concept Experiments
- **Juan Sebastian Flórez**, Juan Daniel Valderrama-Rincon, Luis H. Reyes, Juan C Cruz
- **2:18 Paper 498g:** Invited Talk Bioprocess Design
- Tamara L. Kinzer-Ursem

(499) Advances in Drug Discovery Processes

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 7 Samir Kulkarni, Chair Luke Rogers, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **12:30 Paper 499a:** *In Vitro* biomimetic Tumor Model for High Throughput Drug Screening
- You Li, Xin Xin, Shang-Tian Yang
- **12:55 Paper 499b:** Automated Nanomole-Scale Platform for Rapid Screening and Optimization of Electroorganic Synthesis
- **Yiming Mo**, Girish Rughoobur, Zhaohong Lu, Klavs F. Jensen
- **1:20 Paper 499c:** Virtual Rodents: Design and Translation of Glucose-Responsive Insulins Aided By Pharmacokinetic Modeling
- **Jing Fan Yang**, Xun Gong, Naveed Bakh, Michael Weiss, Michael Strano
- **1:45 Paper 499d:** Combined Synthesis Planning for Synthetic Drugs on the WHO Essential Medicines List
- **Hanyu Gao**, Connor W. Coley, Thomas Struble, Linyan Li, Yujie Qian, William H. Green, Klavs F. Jensen
- **2:10 Paper 499e:** Epitope-Targeted Peptide Immunostimulants to Combat Antibiotic-Resistant Bacteria
- **Matthew N. Idso**, Ajay Akhade, Mario Arrieta-Ortiz, Jimmi Hopkins, Naeha Subramanian, Nitin Baliga, James R. Heath
- 2:35 Paper 499f: Mathematical Modeling and Optimization of the Upstream Monoclonal Antibody Production
- Ou Yang, Marianthi lerapetritou

(500) Advances in Process Design II Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 24 Emre Gençer, Chair Apratim Bhattacharya, Co-Chair Qi Zhang, Co-Chair

Sponsored by: Systems and Process Design

- **12:30** Paper **500a**: Expanding the Scope of Distillation Network Synthesis Using Superstructure-Based Methods *Lingxun Kong*, *Christos T. Marayelias*
- **12:49 Paper 500b:** Application of Trust Region Methods for Optimal Heat Exchanger Network Synthesis a Hybrid Optimization Strategy
- **Saif R. Kazi**, Michael Short, Lorenz T. Biegler
- **1:08** Paper **500c**: Process Design Frameworks for Cost-Effective Small-Scale Processes
- **Akhil Arora**, Jianping Li, Manali Zantye, M. M. Faruque Hasan
- 1:27 Paper 500d: A Novel Method to Compare Chemical Process Flowsheets Chenglin Zheng, Tong Zhang, Nikolaos V. Sahinidis, Jeffrey J. Siirola, Xi Chen
- **1:46** Paper **500e**: Single Shooting Method for Semicontinuous Distillation Design
- **Pranav Bhaswanth Madabhushi**, Thomas A. Adams II
- 2:05 Paper 500f: A Consolidated/ Unified Framework for Computer-Aided Process Synthesis-Intensification — M. M. Faruque Hasan, Rafiqul Gani, Efstratios N. Pistikopoulos
- **2:24** Paper 500g: Simultaneous Optimization of Membrane-Cryogenic Hybrid System for CO₂ Capture and Separation
- Zuwei Liao, Fengqi You
- 2:43 Paper 500h: A Rapid Screening Methodology for Chemical Processes — Jeffrey A. Frumkin, Michael F. Doherty
- (501) Advances in Processing and Handling of Energetic Materials Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 21 Lori J. Groven, Chair Andrew G. Pearsall, Co-Chair

Sponsored by: Energetics

- **12:30 Paper 501a:** Bringing Particle Scale Properties into Descriptions of Energetic Powder Behavior Via the Enhanced Centrifuge Technique
- Caralyn A. Coultas-McKenney, Contessa Norris, Andrew Roginski, Kacie Bradfish, Emma Weiglein, Stephen P. Beaudoin
- **12:50 Paper 501b:** Numerical Simulation of Munitions Response for Fragment IMPACT
- Ruslan S. Mudryy
- **1:10 Paper 501c:** Filled Spherical Composite Particles Prepared By Mechanical Milling
- **Mehnaz Mursalat**, Daniel Hastings, Mirko Schoenitz, Edward Dreizin
- **1:30 Paper 501d:** Influence of Nanoconfinement on the Degradation of CL-20 and HMX
- **Rozana Bari**, Aric Denton, Zachary Fondren, Victor Stepanov, Sindee L. Simon, Gregory B. McKenna

- **1:50 Paper 501e:** Influence of Catalyst on the Mechanochemical Nitration of Toluene
- **Ashvin Kumar Vasudevan**, Edward L Dreizin, Mirko Schoenitz
- **2:10 Paper 501f:** Ignition of Reactive Material Powders in Vicinity of an Electrostatic Discharge
- **Ci Huang**, Mirko Schoenitz, Edward Dreizin
- 2:30 Break
- **2:50** Paper 501h: Synthesis and Characterization of a Biocidal Co-Crystal *Clinton Chapman*, *Lori J. Groven*
- (502) Applications of Data Science in Molecular Sciences II

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Peacock Spring

Johannes Hachmann, Chair Andrew White, Co-Chair Andrew L. Ferguson, Co-Chair

Sponsored by: Applications of Data Science to Molecules and Materials

- **12:30** Paper **502a**: Understanding Photonic Band Gaps in Three Dimensions *Rose Cersonsky*, *James Antonaglia*, *Bradley Dice*, *Sharon C. Glotzer*
- **12:45 Paper 502b:** Learning Structure Identification in Molecular Simulations with a Pointnet
- Ryan DeFever, Colin Targonski, Steven Hall, Melissa Smith, **Sapna Sarupria**
- **1:00** Paper **502c:** Studying the Importance of Preserving Symmetry in Coarse-Grained Alkanes
- **Maghesree Chakraborty**, Andrew White
- 1:15 Paper 502d: Construction of Coarse-Grained Neural Network Potentials for Predicting Water Properties
- **Tarak Patra**, Troy Loeffler, Henry Chan, Subramanian Sankaranarayanan
- **1:30 Paper 502e:** Neural Network Potential for Predicting Bond Dissociation Energies
- Richard A. Messerly
- **1:45** Intermission
- **2:00** Paper 502f: Toward Universal Prediction of Adsorption Isotherms in Metal-Organic Frameworks Using Deep Learning Algorithms
- **Ryther Anderson**, Achay Biong, Diego Gomez Gualdron
- 2:15 Paper 502g: Intensive Chemical Descriptors for Nanoporous Crystalline Materials
- Farhad Gharagheizi, David S. Sholl
- 2:30 Paper 502h: Eigencages: Learning a Latent Space of Porous Cage Molecules
- Arni Sturluson, Melanie Huynh, Arthur York, **Cory Simon**

- 2:45 Paper 502i: Deep Neural Network Learning of Complex Binary Sorption Equilibria from Molecular Simulation Data
- Yangzesheng Sun, Robert F. DeJaco, J. Ilja Siepmann

(503) Atmospheric Chemistry and Physics: Modeling and Field Studies Wednesday, Nov 13, 12:30 PM

Hyatt Regency Orlando, Blue Spring I/II Shunsuke Nakao, Chair Kristina Wagstrom, Co-Chair Marwa El-Sayed, Co-Chair

Sponsored by: Air

- 12:30 Paper 503a: Characterizing Aerosol Liquid Water at Two Contrasting Locations in the Eastern and Western United States
- **Marwa El-Sayed**, Katherine Benedict, Christopher Hennigan, Jeff Collett Ir
- **12:50 Paper 503b:** Chemical Fingerprinting of Particulate Organic Compounds in Fresh Smoke Produced from Burning Individual Western U.S. Wildland Fuels
- **Coty Jen**, Lindsay Hatch, Nathan Kreisberg, Christos Stamatis, Yutong Liang, Robert Weber, John Battles, Scott Stephens, Robert York, Kelley Barsanti, Allen Goldstein
- **1:10** Paper **503c**: Modeling Smog Chamber Experiments: Forward and Inverse
- **Naser G. A. Mahfouz**, Neil M. Donahue
- **1:30** Paper **503d:** Development of a Calibration Chamber to Evaluate the Performance of Low-Cost Particulate Matter Sensors
- **Dylan Kaufman**, Tofigh Sayahi, Kerry Kelly, Tony Butterfield, Pierre Gaillardon, Tom Becnel
- **1:50 Paper 503e:** Comparing Cyclist Air Pollution Exposures in Major Cities in the United States
- Kristina Wagstrom
- **2:10** Paper **503f**: Comparisons and Contrasts of Jet Engine Emissions with Other PM_{2.5} Combustion Sources

 Madhu Singh, Randy Vander Wal
- $\begin{array}{lll} \textbf{2:30 Paper 503g:} & \text{Variations HCHO,} \\ \textbf{NO}_2 & \text{and SO}_2 & \text{Vertical Column Densities} \\ \text{from 2005 to 2017 in Five Countries} \\ \text{Surrounding the Caspian Sea} \end{array}$
- **Mehdi Amouei Torkmahalleh**, Zhuldyz Darynova, Turar Yerkenov, Botagoz Kuspangaliyev, Kamila Altazhanova

(504) Big Data and Applications in Advanced Modeling and Manufacturing

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 27 Mona Bavarian, Chair Sudarshan Ganesh, Co-Chair

Sponsored by: Next-Gen Manufacturing

12:30 Welcoming Remarks

- **12:35** Paper **504a**: Coefficient-Setups for Subset Selection in Model Structure Identification Problems Using MILP/MIQP *Jeffrey D. Kelly, Brenno C. Menezes, Robert E. Franzoi*
- **12:53 Paper 504b:** Utility Functions for Bayesian Design of Tests for Fault Detection and Isolation
- **Evangelos K. Stefanidis**, George M. Bollas
- **1:11** Paper 504c: Nonlinear Observer Design for Process Monitoring in the Presence of Fast and Slow Modes
- Zhaoyang Duan, Costas Kravaris
- 1:29 Paper 504d: Model-Predictive Safety: Min-Max Optimization to Calculate the Most Aggressive Control Actions and the Worst-Case Uncertainties
- **Masoud Soroush**, Leila Samandari Masooleh, Ulku Oktem, Warren D. Seider, Jeffrey E. Arbogast
- 1:47 Paper 504e: Utilization of Advanced Analytics to Monitor Catalyst Health in an Ethylene Oxide Reactor — Şahin Sarrafi, Hasan Sildir, Yaşar S. Kahak
- 2:05 Paper 504f: Exploring the Role of System Knowledge in Data Analytics Using an liot-Enabled Smart Manufacturing Testbed
- **Devarshi Shah**, Jesus Flores-Cerrillo, Jin Wang, Q. Peter He
- 2:23 Paper 504g: The Nature of Fault-Space Classification By Neural Networks — Laya Das, Abhishek Sivaram, Venkat Venkatasubramanian
- **2:41** Paper 504h: A Novel Data-Driven Causality Digraph Modeling of Large-Scale Industrial Processes
- Feifan Cheng, Jinsong Zhao

(505) Biomaterials in Industry and the Clinic

Wednesday, Nov 13, 12:30 PM
Hyatt Regency Orlando, Celebration 16
Abhinav P. Acharya, Chair
Latrisha K. Petersen, Co-Chair
Jerome Unidad, Co-Chair
Ashish Kulkarni, Co-Chair

Sponsored by: Biomaterials

- **12:30 Paper 505g:** Quantum Dots for Clinical Cancer Diagnostics: A Translation Story
- Jessica O. Winter
- 1:12 Paper 505a: Development of Safety and Efficacy Models to Support Consumer-Focused Claims for Novel First-Aid Materials
- Katie Wlaschin, Jana Ninkovic, George Griesgraber, Semra Colak Atan, Alexi Young, Junia Pereira, Michael Solberg, Delony Langer-Anderson
- **1:30 Paper 505b:** Preparation and Validation of a Biopolymer-Based Coating on Titanium Prosthesis for Preventing Infection in Orthopedics Implants
- Antonio Tabernero, Álvaro González-Garcinuño, **Eva M. Martín del Valle**

- 1:48 Paper 505c: Development and Commercialization of MicroLyte® Ag Antimicrobial Matrix: A Start-up's Journey
- **Gaurav Pranami**, Ankit Agarwal, Eric C. Crawford, Tyler B. Nelson, Anna M O'Keefe
- 2:06 Paper 505d: Heparin/Collagen Coatings Improve Human Mesenchymal Stromal Cell Response to Interferon Gamma
- **David Castilla-Casadiego**, José R. García, Andres Garcia, Jorge Almodovar
- 2:24 Paper 505e: Solution Deposited Hydroxyapatite Coatings for Titanium Based Orthopedic Implants
- **Rajendra Kasinath**, Stephanie Vass, Bryan Smith
- **2:42 Paper 505f:** Computationally-Designed Nanomaterials for Cancer Immunotherapy
- Ashish Kulkarni

(506) Catalysis for Nitrogen Chemistry II: Plasma-Enhanced and Other Non-Thermal Approaches for N2 Activation

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom D Prateek Mehta, Chair Ashley M. Pennington, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 506a:** Nitrogen Activation Under Non-Thermal Stimulation
- Prateek Mehta, Patrick Barboun, Francisco Herrera, David Go, Jason C. Hicks, **William F. Schneider**
- **12:48 Paper 506b:** Revealing Plasma Catalysis Mechanisms of N_2 Reduction Using an in-Situ FTIR Dielectric Barrier Discharge Reactor
- **Lea Winter**, Jingguang G. Chen
- **1:06** Paper 506c: Plasma-Enhanced Catalytic Ammonia Synthesis As a Technology for Decentralized Power-to-Ammonia Applications
- Kevin Hendrik Reindert Rouwenhorst, Leon
- Lefferts 1:24 Paper 506d: Plasma Aided Nitrogen Fixation: Electrocatalysis vs Catalysis
- **R. Sharma**, H. Patel, V. Kyriakou, U. Mushtaq, A. Pandiyan, S. Welzel, M.C.M. van de Sanden, M. Tsampas
- **1:42** Paper **506e**: Plasma-Based Electrolytic Synthesis of Ammonia from Nitrogen and Water
- Ryan Hawtof, Souvik Ghosh,
 Evan Guarr, R. Mohan Sankaran, Julie
 N. Renner
- 2:00 Paper 506f: Towards Understanding Plasma-Assisted Catalytic Enhancement of Ammonia Synthesis over Supported Metal Catalysts
- **Patrick Barboun**, Prateek Mehta, Francisco Herrera, David Go, William F. Schneider, Jason C. Hicks

- **2:18 Paper 506g:** Transcending the Volcano Plot: Enhancing NH₃ Synthesis with Dynamic Catalysis
- M. Alexander Ardagh, Shizhong Liu, Gerhard R. Wittreich, Omar A. Abdelrahman, Qi Zhang, Dionisios G. Vlachos, Paul Dauenhauer
- 2:36 Paper 506h: Photocatalytic Nitrogen Fixation: Insights from Computational Chemistry and Surface Science — Andrew Medford, Benjamin Comer, Marta Hatzell

(507) Cells, Organs, and Labs on a Chip Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 1 Ryan Koppes, Chair Heather Fahlenkamp, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

Adriana San-Miguel, Co-Chair

- **12:30 Paper 507a:** Glycosylation-on-a-Chip for Tunable Cell-Free Synthesis of Glycoproteins
- **Alicia K. Aquino**, Zachary A. Manzer, Susan Daniel, Matthew P. DeLisa
- **12:48** Paper **507b**: Biomanufacturing of GBM Tumor Microenvironment Using a Small Scale Bioreactor
- **Seungjo (Joe) Park**, Yonghyun (John) Kim
- 1:06 Paper 507c: Fabrication and Maturation of Cancer Spheroids (Micro-Tumors) in a 3D-Printed Continuous Stirred Tank Mini-Reactor (CSTmR)
- Salvador Gallegos-Martínez, Itzel Montserrat Lara-Mayorga, Brenda Giselle Flores-Garza, Ingrid Anayo-Morales, Germán García-Martínez García-Martínez, Christian Carlos Mendoza-Buenrostro, Juan Felipe Yee-de León, Ciro Angel Rodríguez-González, Grissel Trujillo-de Santiago, Mario Moisés Álvarez
- **1:24** Paper **507d**: Exploring the Role of Pericytes in Blood-Brain Barrier Maintenance Using hiPSC-Derived 2D and 3D *in Vitro* models
- **John Jamieson**, Raleigh Linville, Yuan Yuan Ding, Daniel Soto, Sharon Gerecht, Peter C. Searson
- 1:42 Paper 507e: Continuous, High Throughput Microfluidic Device to Monitor Circulating Tumor Cells in Cancer Patients
- Tae Hyun Kim, Yang Wang, C. Ryan Oliver, Douglas Thamm, Laura Cooling, Costanza Paoletti, **Kaylee Smith**, Sunitha Nagrath, Daniel Hayes
- 2:00 Paper 507f: Predicting Progression-Free Survival and Recurrence Time of Primary Glioblastoma Using a Microfluidic Invasion Network Device
- Bin Sheng Wong, Sagar R. Shah, Christopher L. Yankaskas, Alfredo Quiñones-Hinojosa, Konstantinos Konstantopoulos

- **2:18** Paper **507g**: Invited: Rapid Prototyping of Multilayered, Thermoplastic, Patient-Derived Organs-on-Chips
- Sanjin Hosic, David Breault, Shashi Murthy, Ryan Koppes, **Abigail Koppes**

(508) Challenges and Best Practices in Technology Commercialization Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 18 Ha Dinh, Chair Yiling Xu, Co-Chair

Sponsored by: Technology Transfer and Manufacturing

- **12:30 Paper 508a:** Findings from MTO Commercialization Don't Forget about the Small Stuff
- Joe Montalbano
- **1:00** Paper **508b**: De-Risking Technology Development and Scale-up Efforts Effectively in Fuel and Chemical Processes
- **Greg DiCosola**, Dan Parker, Matt Schneider, Bernardo Flores
- **1:30 Paper 508c:** Can Outsourcing R&D Balance Myopic Business Management?
- Michael Bradford
- **2:00 Paper 508d:** Succeeding at Innovation: Generating Value from New Technology at Each Stage of Development and Implementation
- Howard Stamato
- **2:30 Paper 508e:** Heat Transfer Coefficient in Two Phase Liquid-Solid Fluidized Bed
- Jamal M. Ali Sr.

(509) Characterization of Continuous Drug Product Unit Operations Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 6 Pallavi Pawar, Chair Sarang Oka, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **12:30** Paper **509a**: A Piecewise Parametric Model for Open Loop Screw Feeder Flow Rates
- **Brad Johnson**, Salvador García-Muñoz, Maitraye Sen, Joshua Hanson, David Slade, Nick Sahinidis
- **12:51 Paper 509b:** Hybrid Theoretical-Empirical Approach to Modelling of Twin Screw Feeders for Continuous Tablet Manufacturing
- Davide Bascone, Federico
 Galvanin, Nilay Shah, Salvador García-Muñoz
- **1:12** Paper 509c: Continuous Twin-Screw Powder Feeding a Crossroad for Continuous Process Development
- Theresa R. Hörmann, Julia Kruisz, Michela Beretta, Eva Faulhammer, Wen-Kai Hsiao, Johannes G. Khinast

- **1:33 Paper 509d:** Continuous Mixing Technology: Design Optimization with Discrete Element Simulations
- Peter Toson, **Pankaj Doshi**, Eva Siegmann, Johannes G. Khinast, Daniel O. Blackwood, Ashwinkumar Jain, Alexandre Bonnassieux, Kai Lee, David Wilsdon, James Kimber, Dalibor Jajcevic
- 1:54 Paper 509e: Optimization of Batch High Shear Granulation and Transfer to a Continuous Granulation Process: A Case Study of Metoprolol Succinate ER Tablets
- Lalith Kotamarthy, Xin Feng, Alaadin Alayoubi, Thomas O'Connor, Muhammad Ashraf, Celia N. Cruz, Ahmed Zidan
- 2:15 Paper 509f: Dampening Effect of Feedrate Variation By Downstream Unit Operations in Pharmaceutical Continuous Manufacturing
- **Tianyi Li**, James V. Scicolone, Benjamin Glasser, Fernando J. Muzzio
- 2:36 Paper 509g: Investigation of Electric Capacitance-Based and X-Ray-Based Sensors for Real-Time Mass Flow Rate Monitoring in Continuous Tablet Manufacturing
- **Yan-Shu Huang**, Sudarshan Ganesh, Qussai Marashdeh, Christopher Zuccarelli, Zoltan K. Nagy, Gintaras V. Reklaitis

(510) Chemical Engineering Applications in Cancer

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 12/13

Mikhail Skliar, Chair Jamie B. Spangler, Co-Chair

Sponsored by: Chemical Engineers in Medicine

- **12:30** Paper 510a: Fractionation of Extracellular Vesicles into Molecularly Homogeneous Subpopulations

 Mikhail Skliar
- **12:51 Paper 510b:** Cancer Progression As a Transport Problem
- **Adeyinka Lesi**, David Rumschitzki
- **1:12 Paper 510c:** Reengineering the Tumor Microenvironment for Immunotherapy
- John D. Martin
- 1:33 Paper 510d: Biogenic Metallic Nanoparticles. from Microbiological Biofactories to Nanometric Trojan Horses
- **David Medina**, Ada Vernet Crua, Junjiang Chen, Thomas J. Webster
- **1:54 Paper 510e:** Characterization of Extracellular Vesicles By Atomic Force Microscopy
- Mikhail Skliar, Vasily Chernyshev
- 2:15 Paper 510f: Targeted Pegylated Mesoporous Silica Nanoparticles for the Delivery of Curcumin in a Pancreatic Cancer Animal Model: Inhibition of Both Tumor Growth and Metastasis

 R S Prabhuraj, Arijit Mal, Snehal K Valvi, Rohit Srivastava, Abhijit De,

Rajdip Bandyopadhyaya

- **2:36** Paper **510g:** Data Analytics and Optimization for Minimization of Chemotherapeutic Toxicity
- Katherine Schmidt, Alex D'Aloia, Purnima Kodate, **Kirti M. Yenkie**

(511) Chemical Safety and Sustainability

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Regency Ballroom T

William M. Barrett, Chair Konstantinos Kokosimos, Co-Chair

Sponsored by: Sustainability Science and Engineering

- **12:30 Paper 511a:** Effect of Parameters on Sweet Potato Dust Explosion
- Chunyan Chen
- **12:50 Paper 511b:** Risk Characterization of Cadmium Based on Human Biomonitoring Data
- **Spyros Karakitsios**, Ioannis Petridis, Dimosthenis Sarigiannis
- **1:10 Paper 511c:** Risk Assessment of Phthalates and Dinch Starting from Human Biomonitoring Data
- **Spyros Karakitsios**, Ioannis Petridis, Dimosthenis Sarigiannis
- **1:30 Paper 511d:** Aerosol Explosion Studies Using Modified Dust Explosion Apparatus
- **Shuai Yuan**, Joseph Sang-II Kwon, Chad Mashuga
- 1:50 Paper 511e: A Novel Quantitative Chemical Reactivity Rating System Design By Machine Learning Methodology
- **Lin Zhao**, Wen Zhu, Shuai Yuan, Mustafa Akbulut
- **2:10 Paper 511f:** Immersive Digital Experiences for Process Safety Decision Making
- **Cheryl A. Bodnar**, Matthew Cooper, Daniel D. Burkey, Daniel Anastasio

(512) Community-Based Water Treatment Innovations

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Rainbow Spring I/II

Steven T. Weinman, Chair Sage R. Hiibel, Co-Chair

Sponsored by: Water

- **12:30 Paper 512a:** Enhanced Virus Removal in a Practical Sand Filter
- Andrew Pei, Laxmicharan Samineni, Louise Kuehster, Roman Dickey, Huiran Wang, Paula Espinoza, Ratul Chowdhury, Costas Maranas, Manish Kumar, Stephanie B. Velegol
- **12:50 Paper 512b:** Fairness-Guided Design of Water Distribution Systems for Agricultural Lands
- Aurora del Carmen Munguía-López, Eusiel Rubio-Castro, José María Ponce-Ortega, Victor M. Zavala

- 1:10 Paper 512c: Experimental Study of the Potential of Nano-Fibrous Membranes in Water Treatment Systems for Rural Communities
- **Pooja Yadav**, Vivek Kumar, Ramin Farnood
- 1:30 Intermission
- **1:50 Paper 512d:** Effects on Incubating Functional Bacteria with Different-Sizes Microplastics: An Unexpected Increase of COD Removal Rate with Presence of Microplastics
- Mu Lin. J. Paul Chen
- 2:10 Paper 512e: Analyzing Spinach Growth Using Vertical Garden Techniques and Local Water Sources for Urban Gardens
- Julia Ashlyn Manzella, Mariam Massoud, Mohamed K. Mostafa, Ahmed S. Mahmoud, **Robert W. Peters**
- 2:30 Paper 512f: Dynamic Modeling of Advanced Wastewater Treatment Plants Using Biowin for Model-Based Control — Komal Rathore, Aaron Driscoll, Kyle Cogswell, Aydin K. Sunol, Gita Iranipour,

(513) Complex Fluids

Luke Mulford

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom M

Michelle A. Calabrese, Co-Chair Samanvaya Srivastava, Co-Chair

Sponsored by: Fluid Mechanics

- **12:30 Paper 513a:** Experimental Decomposition of the Rheological Responses of Elastoviscoplastic Materials
- **Simon Rogers**, Gavin Donley
- **12:45** Paper 513b: On the Extensional Rheology of a Particle-Laden Viscoelastic Solution

 Anika Jain
- **1:00 Paper 513c:** Simulating Transport in Particle-Polymer Solutions with Multi-Particle Collision Dynamics
- Renjie Chen, Jacinta C. Conrad, Jeremy C. Palmer
- **1:15** Paper **513d**: Understanding the Effect of Solution Spinning Processing Parameters on the Structure and Properties of Carbon Nanotube Fiber
- Lauren Taylor, Oliver Dewey, Matteo Pasquali
- 1:30 Paper 513e: The Influence of Carrier Polymer on the Microstructure and Rheology of Catalyst Inks for Electrospun Proton Exchange Membrane Fuel Cell Electrodes
- **Sunilkumar Khandavalli**, Sadia Kabir, Samrat Sur, Jonathan P. Rothstein, K.C. Neyerlin, Michael Ulsh, Scott A. Mauger
- **1:45** Paper **513f**: Structural Breakdown in Sheared Carbon Black Suspensions *Julie B. Hipp, Norman J. Wagner*

- 2:00 Paper 513g: Recovery Rheology Via Rheo-SANS: Application to Step Strains Under out-of-Equilibrium Conditions
- **Johnny Ching-Wei Lee**, Lionel Porcar, Simon Rogers
- 2:15 Paper 513h: Bi-Disperse Multiple Particle Tracking Microrheology for Characterizing Length Dependent Rheological Properties
- Matthew Wehrman, Seth Lindberg, John McGlynn, **Kelly M. Schultz**
- 2:30 Paper 513i: Enabling Rheological Analysis of Complex Fluids at the Pointof-Need
- Jose C. Contreras-Naranjo, Victor M. Ugaz
- 2:45 Paper 513j: System Size Dependence of the Structure and Rheology in a Sheared Lamellar Liquidcrystalline Medium
- **—Viswanathan Kumaran**, Someshwar Jaiu

(514) CO₂ Capture By Adsorption Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Manatee Spring II

Youssef Belmabkhout, Chair

Sponsored by: Adsorption and Ion Exchange

- 12:30 Paper 514a: An Adsorbent Screening Tool with Integrated Process Economics for Carbon Capture By PVSA — David Danaci, Niall Mac Dowell, Camille Petit
- **12:52 Paper 514b:** Bi-Functionalized lonic Liquid/MOF Composite Material for Efficient Carbon Dioxide Capture and Conversion
- Liwei Sun, Shaokun Tang
- 1:14 Paper 514c: Capture and
 Methanation of CO₂ Using Sodium
 Promoted MgO Based Catalytic Sorbent
 Sang Jae Park, Christopher W.
 Jones
- **1:36 Paper 514d:** Amine-Based Latex Coatings for Indoor Air CO₂ Control in Commercial Buildings
- Anirudh Krishnamurthy, Ali Rownaghi, Thomas Schuman, **Fateme Rezgei**
- **1:58** Paper **514e**: A History of Temperature Swing Adsorption Compression for Use in Spacecraft *TRA-My Richardson*, *Darrell Jan*
- 2:20 Paper 514f: Combined Capture and Utilization of CO₂ in Ethylene Production over Dual-Function Materials Ahmed Al-Mamoori, Ali Rownaghi, Fateme Rezaei
- 2:42 Paper 514g: Batch Adsorber Analogue Model Based Screening of Large Adsorbent Databases for Post-Combustion CO₂ Capture
- Vishal Subramanian Balashankar,
 Arvind Rajendran

(515) CO₂ Capture, Utilization, and Disposal: Key to Clean Energy Production

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 29/30 Chakravarthy Sishtla, Chair Nagasree Garapati, Co-Chair

Sponsored by: Transport and Energy Processes

- 12:30 Paper 515a: Highly Efficient Sorbent Systems for Carbon Capture — Ambalavanan Jayaraman, Gokhan Alptekin, Dave Gribble, Michael Bonnema, Chakravarthy Sishtla
- **12:48** Paper **515b:** Transformational Graphene Oxide-Based Membrane Process for Post-Combustion CO₂ Capture
- Shiguang Li, Miao Yu
- **1:06 Paper 515c:** A Computational Investigation of Hollow Fibers for Carbon Capture
- **Grigorios Panagakos**, Surendar Venna, David E. Huckaby, David Hopkinson
- 1:24 Paper 515d: Water Lean Amine-Based Solvents for Carbon Dioxide Capture
- **Phillip K. Koech**, Manh-Thuong Nguyen, Deepika Malhotra, David J. Heldebrant, Andy J. Zwoster, Vassiliki-Alexandra Glezakou, Richard Zheng, Roger Rousseau
- **1:42** Paper **515e**: CO₂ Absorption in Amines Using SiO₂ Nanoparticles in Instantaneous Regime
- **Tejeswi Ramprasad**, Akkihebbal K. Suresh
- **2:00** Paper 515f: Plant-Wide Optimization of a Moving Bed Process for CO₂ Capture Using a Micro-Encapsulated Solvent
- **Goutham Kotamreddy**, Ryan Hughes, Debangsu Bhattacharyya, Joshuah Stolaroff, Benjamin P. Omell, Michael S. Matuszewski
- 2:18 Paper 515g: CO₂ Utilization Via Chemical Looping Dry Reforming: Process Modeling and Systems Analysis — Hari C. Mantripragada, Götz Veser
- 2:36 Paper 515h: Design Development of an Integrated Reforming and Gasification Technology for Syngas Production
- **Umer Zahid**, Hussain Al-Ibrahim

(516) Data Science Education in Chemical Engineering Panel Discussion

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Manatee Spring I

Leo H. Chiang, Chair Victor M. Zavala, Co-Chair

Sponsored by: Miscellaneous

12:30 Paper 516a: Industry Perspective — *Lloyd Colegrove*

12:48 Paper 516b: CACHE Perspective — *Richard D. Braatz*

1:06 Paper 516c: Chemical Engineering Department Chair Perspective

- Sharon C. Glotzer

1:24 Paper 516d: Chemical Engineering Data Science Class Instructor Perspective I

- Curtis Martin

1:42 Paper 516e: Chemical Engineering Data Science Class Instructor Perspective II

— Joe Qin

2:00 Panel Discussion

(517) Developments in Extractive Separations: Solvents

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Barrel Spring II George S. Goff, Chair David C. Cantu, Co-Chair

Sponsored by: Extractions

- **12:30** Paper **517a:** Liquid-Liquid Based *in Situ* Recovery Systems Enhance Bioproduct Production and Enable New Bioprocesses
- **Eric M. Karp**, Patrick Saboe, Hanna Monroe, William Michener, Lorenz Manker, Stefan Haugen, Robert S. Nelson, Davinia Salvachua, Violeta Sànchez i Nogué
- **12:55** Paper **517b**: Design and Performance of Amine Based Solvents *Matthaeus Siebenhofer*, *Annika Grafschafter*
- **1:20 Paper 517c:** Direct Numerical Simulation of Liquid-Liquid Droplet Interactions
- Patrick Zimmermann, Tim Zeiner
- **1:45** Paper 517d: Effects of Different Additives on Fluid Dynamics and Mass Transfer in Single Drop Extraction
- Joschka M. Schulz, Marc Petzold, **Matthias Kraume**
- **2:10** Paper 517e: Unifac Correlated Parameters for Liquid-Liquid Equilibrium Prediction of Ternary Systems Related to Biodiesel Production Process
- **Mario Andrés Noriega**, Paulo C. Narvaez

(518) Diffusion in Polymers Wednesday, Nov 13, 12:30 PM

Hyatt Regency Orlando, Celebration 5 Bryan S. Beckingham, Chair Charles E. Sing, Co-Chair

Sponsored by: Polymers

- **12:30** Paper **518a:** Accelerated Predictions of Small-Molecule Diffusion in Polymers
- Robert M. Elder, David M. Saylor
- **12:45 Paper 518b:** Impact of Humidity on Gas Transport in Polybenzimidazoles
- **Joshua D. Moon**, Hailun Borjigin, Ran Liu, Ronald M. Joseph, Judy S. Riffle, Benny D. Freeman, Donald R. Paul
- **1:00 Paper 518c:** Sorption and Diffusion By 3D Printable Polymeric Materials
- **Hom Sharma**, Jeremy Lenhardt, Yunwei Sun, Elizabeth Glascoe

- **1:15 Paper 518d:** Measurements of Methanol Permeation Rates across Thermoset Organic Coatings
- **Ting Wang**, Shicong Luo, Claus Erik Weinell, Kim Dam-Johansen, Søren Kiil
- **1:30 Paper 518e:** Tuning Transport and Segmental Dynamics in Ionomer Nanocomposites Via Membrane-Nanoparticle Interactions
- **Eric M. Davis**, Apoorv Balwani, Allison Domhoff
- **2:00** Paper **518f**: Study of Lithium Salt Dissociation and Diffusion in Block Copolymer Via Spectroscopy
- **Kyoungmin Kim**, Daniel T. Hallinan *Ir*.
- 2:15 Paper 518g: Impact of Polyether Polarity on Ionic Conductivity and Segmental Dynamics in Salt Doped Systems
- Malgorzata Chwatko, Bill Wheatle, Alysha Helenic, Venkat Ganesan, Nathaniel A. Lynd
- **2:30** Paper 518h: Molecular Understanding of Polyamide Membrane in Desalination at Equilibrium and Nonequilibrium States Using Molecular Simulations
- Md Symon Jahan Sajib, Tao Wei
- **2:45** Paper **518i**: Elucidating the Relationship between the States of Water and Transport Properties of Ions in Swollen Polymer Networks
- Thien Tran, Chen Lin, Haiqing Lin

(519) Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions I

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom I Hong Yang, Chair Rachael H. Rothman, Co-Chair Gang Wu, Co-Chair

Sponsored by: Electrochemical Fundamentals

- **12:30 Paper 519a:** U.S. Doe Reversible Fuel Cell R&D to Support Grid-Scale Energy Storage (invited)
- **Simon T. Thompson**, David Peterson, Dimitrios Papageorgopoulos
- **1:00** Paper **519b:** Reversible Fuel Cells -Challenges and Perspectives for Energy Conversion (invited)
- Hui Xu, Cortney Mittelsteadt
- 1:20 Paper 519c: Enhanced Catalyst Durability in PtCo Fuel Cell Catalysts Using Atomic-Level Ordering (invited) — Chenyu Wang, Dongguo Li, Vijay Kumar, David Cullen, Karren L. More, Jacob S. Spendelow
- **1:40** Paper **519d:** Renewable Power to Synfuels: Building on Solid Oxide Electrolysis Advances Developed for the Mars₂₀₂₀ Mission
- **Joseph J. Hartvigsen**, S. Elango Elangovan, Lyman Frost

- 2:00 Paper 519e: Improving the Efficiency of High Temperature Electrolysis of Carbon Dioxide in an SOC Ann V. Call, Thomas Holmes, Tom Butterworth, Pratik Desai, William B. Zimmerman, Rachael H. Rothman
- **2:20 Paper 519f:** Water Electrolysis without Membranes: Opportunities and Limitations
- Daniel Esposito

2:40 Paper 519g: Understanding HER/ HOR Kinetics through Ru(OH)x Surface Decoration on Pt Single Crystals — Saad Intikhab, Luis Rebollar, Maureen H. Tang, Joshua Snyder

(520) Emerging Junior Investigator Open Innovation Forum (Invited Talks)

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 10 Su Ha, Chair Younjin Min, Co-Chair Yoonjee Park, Co-Chair

Sponsored by: International Committee

- **12:30** Paper **520a**: Enhancing Hydraulic Fracturing Productivity Via Model-Based Feedback Control *Joseph Sang-Il Kwon*
- **12:50 Paper 520b:** In Situ Grown Metal Nanoparticle Catalysts: Properties and Control
- Tae-Sik Oh
- 1:10 Paper 520c: MFI-Type
 Zeolite Membrane Reactor for High
 Temperature Ethane Dehydrogenation
 Seok-Jhin Kim
- **1:30** Paper **520d**: Can Phosphorus-Doped Graphene be a Good Anode for Na-Ion Batteries?: A First-Principles Study
- Eunsu Paek
- **1:50 Paper 520e:** Hydrogen Storage for PEM Fuel Cell Applications
- Hyun-Tae Hwang
- **2:10** Paper 520f: Eradicating Antibiotic-Tolerant Bacteria and Biofilms By Antimicrobial Proteins Produced By Cell-Free Protein Synthesis
- Seok Hoon Hong
- **2:30 Paper 520g:** Hanwha Travel Award Flash Presentations
- Hyunmin Yi

(521) Engineering the Tissue and Cell Microenvironment I: Promoting Functionality and Repair

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 14 Samira M. Azarin, Chair Tadas Kasputis, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **12:30 Paper 521a:** Next-Generation Neurovascular Models Built from Human iPSCs
- Emma Neal, Shannon Faley, Brian O'Grady, Kylie Balotin, Leon Bellan, **Ethan S. Lippmann**

- 12:48 Paper 521b: Matrix Remodeling Enhances the Differentiation Capacity of Neural Progenitor Cells in 3D Hydrogels — Christopher M. Madl, Bauer L. LeSavage, Ruby E. Dewi, Kyle Lampe, Sarah C. Heilshorn
- **1:06** Paper **521c:** Functionalization of Brain Region-Specific Spheroids with Isogenic Microglia-like Cells
- Liqing Song, Xuegang Yuan, Zachary Jones, Cynthia Vied, Yu Miao, **Mark Marzano**, Jingjiao Guan, Teng Ma, Yi Zhou, Yan Li
- 1:24 Paper 521d: Engineering 3D Silk Tissue Culture Platforms for Skeletal Muscle Repair
- Raul G. Cruz Quintero, Schuyler S. Link, Lauren D. Black III, David L. Kaplan, Whitney L. Stoppel
- 1:42 Paper 521e: A Balanced Charged Immune-Evasive Hydrogel for Rapid and Long-Term Glycemic Regulation in T,DM Mice
- **Yingnan Zhu**, Jiamin Zhang, Lei Zhang
- **2:00** Paper **521f**: Developing a 3D Niche Microenvironment to Improve Stem Cell-Derived β-Cell Maturation for Treatment of Type 1 Diabetes
- **Richard Youngblood**, Daniel Clough, Lonnie Shea
- 2:18 Paper 521g: Invited: When Cells Meet: Rules of (cell) Engagement in Cancer Progression and Tissue Engineering

 Anand Asthagiri

(522) Estimation and Control Under Uncertainty

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 25 Joseph Scott, Chair Zhenyu Wang, Co-Chair

Sponsored by: Systems and Process Control

- **12:30 Paper 522a:** Comparison of Uncertainty Propagation Methods for Output Moment Estimation
- **Samira Mohammadi**, Selen Cremaschi
- **12:49 Paper 522b:** A New Approximate Method for Rapid Estimation of Probability Distributions
- **Francesco Rossi**, Linas Mockus, Gintaras Reklaitis
- **1:08** Paper 522c: A Tube-Based Strategy for Robust Control Synthesis of Periodic Processes
- **Mario Eduardo Villanueva**, Benoit Chachuat, Boris Houska
- 1:27 Paper 522d: Adaptive Stochastic Predictive Control with Recursive Subspace Identification and Learning — Iman Hajizadeh, Mohammad Reza Askari, Ranjeet Kumar, Victor M. Zavala, Ali Cinar
- **1:46** Paper **522e:** Stochastic Design Optimization and Control of Modular Membrane Reactor Units
- **San Dinh**, Fernando V. Lima

- **2:05** Paper **522f:** Benchmarking Stochastic and Deterministic MPC: A Case Study in Stationary Battery Systems
- Ranjeet Kumar, Jordan Jalving, Victor M. Zavala
- 2:24 Paper 522g: Contingency Planning for Fault Tolerance in Robust Nonlinear MPC
- **Tor Aksel N. Heirung**, Joel Paulson, Ali Mesbah
- 2:43 Paper 522h: Integrating Machine Learning-Based Sensing with Model Predictive Control
- Helen Durand

(523) Fermented Food and Beverages

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 9 David E. Block, Chair

Sponsored by: Food Innovation and Engineering

- **12:30 Paper 523a:** Characterization of New Hop Varieties and Beers in Support of New Mexico Craft Brewing Industry
- **Catherine E. Brewer**, Hanah Rheay, Jacob Usrey, Stephen Taylor, Kevin Lombard
- **12:55 Paper 523b:** Presentation Title TRD
- Konrad Miller
- **1:20 Paper 523c:** Presentation Title TBD *Andrew MacIntosh*
- **1:45 Paper 523d:** Presentation Title TBD *Chris Curtin*
- **2:10 Paper 523e:** Presentation Title TBD
- **2:35 Paper 523f:** Presentation Title TBD

(524) Fluid Particle Separation in Energy and Environmental Systems Wednesday, Nov 13, 12:30 PM

Hyatt Regency Orlando, Coral Spring I/II Isaac K. Gamwo, Chair Seyi Odueyungbo, Co-Chair

Sponsored by: Fluid-Particle Separations

- 12:30 Paper 524a: Influence of Nanoparticle Wettability on Absorption and Desorption Mass Transfer Rates at Elevated Pressure in a Simple Hydrocarbon System
- **Michael Miranda**, Ashwin Kumar Yegya Raman, Sayeed Mohammad, Clint Aichele
- **12:50 Paper 524b:** Measuring Crystallization Kinetics of Sparingly Soluble Salts from Supersaturated Waters Using CSTRs-in-Series: Studies with CaCO₃
- Sankaranarayanan Ayyakudi Ravichandran, Jordan Krist, Dakota Edwards, Saied Delagah, John Pellegrino
- **1:10** Paper **524c:** Assessment of Oil Fouling By Oil-Membrane Interaction Energy
- Henry J. Tanudjaja, Begum Tanis-Kanbur, **Jia Wei Chew**

- **1:30** Paper **524d:** Experimental and Numerical Analysis of the Flow in a Filter Press
- Ivhan M. K. Tafner, Eduard R.S. Sasse, **Marcela Kotsuka da Silva**, Leonardo M. Rosa, Jaci C. S. C. Bastos, Vinicyus R. Wiggers, Henry França Meier

(525) Fuel and Energy Decarbonization

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Regency Ballroom U

William M. Barrett, Chair Eric Tan, Co-Chair

Sponsored by: Sustainable Energy

- **12:30** Paper **525a:** Hydrogen Export Industry in Australia: Requirements of Further Technical Research
- Saif al Ghafri, Eric F. May
- **12:55** Paper **525b**: The Role and Value of Negative Emissions Technologies in Decarbonising the Energy System
- **Habiba A. Daggash**, Niall Mac Dowell, Clara F. Heuberger
- **1:20** Paper **525c**: Enviro-Economic Assessment of Electrochemical Routes to Syngas Production
- **Andrea Bernardi**, Daniel F. Rodriguez-Vallejo, Gonzalo Guillén-Gosálbez, Benoit Chachuat
- 1:45 Paper 525d: Performance Evaluation of Waste Biomass to Energy with Carbon Capture and Storage Systems
- Qi Dana
- **2:10** Paper **525f**: Comparison of Processes for Producing OME, an Efficient, Economic, and Sustainable E-Fuel?
- **Jannik Burre**, Dominik Bongartz, Sarah Deutz, André Bardow, Alexander Mitsos
- **2:35 Paper 525g:** CZTS Study Using Electrodeposition
- Thaier Alawadh

(526) Fuel Processing for Hydrogen Production

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Challenger 41/42

Dushyant Shekhawat, Chair Daniel J. Haynes, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

- **12:30 Paper 526a:** Methane Pyrolysis with a Molten Cu-Bi Alloy Catalyst
- Clarke Palmer, Maryam Tarazkar, Henrik Kristoffersen, John Gelinas, Michael Gordon, Horia Metiu, Eric W. McFarland
- **12:47** Paper **526b**: Exploring Thermodynamic and Efficiency Trade-Offs in a High-Pressure Chemical Looping Hydrogen Production System *Mandar Kathe, Fanhe Kong, L.-S. Fan, Melanie Gross*

- **1:04 Paper 526c:** Hydrogen Enriched Syngas through Calcium Looping Gasification of Biomass
- Shakirudeen Salaudeen, **Animesh Dutta**, Bishnu Acharya
- **1:21 Paper 526d:** Hydrogen Production from Methane Cracking in a Fluidized Bed Process
- **Martin Keller**, Akimitsu Matsumura, Atul Sharma
- 1:38 Paper 526e: Fe₂O₃/CaO-Ca₁₂Al₁₄O₃₃ Multifunctional Catalyst in Sorption Enhanced Chemical Looping Reforming of Ethanol Combined with Water Splitting for Hydrogen Production
- Janenipa Saupsor, Suwimol Wongsakulphasatch, Pattaraporn Kim-Lohsoontorn, Palang Bumroongsakulsawat, Worapon Kiatkittipong, Sakhon Ratchahat, Sumittra Charojrochkul, Jinlong Gong, Suttichai Assabumrungrat
- **1:55** Paper **526f**: Longevity Study of Microscale Non-Thermal Plasma Reforming of Methane to Higher Hydrocarbons and Syngas
- Ian Reddick, Omar Mohamed, Ryan Collin, Matthew Coblyn, Yu Miao, Alexandre Yokochi, Goran Jovanovic, Nick AuYeung
- 2:12 Paper 526g: Reducing Carbon Emissions through Novel Hydrogen Sulfide Processing Strategies to Produce Hydrogen Gas
- Ryan J. Gillis, William H. Green
- 2:28 Paper 526h: Hydrogen Injection in Natural Gas Pipelines for Decarbonization of Power Sector in New York State
- Stephanie Taboada, Christopher Cavanagh, McKenzie Schwartz, **Devinder Mahajan**
- 2:44 Paper 526i: Hydrogen Production System Using SOEC - Evaluation of the Energy By Long-Term Operation — Naomi Tsuchiya, Hisao Ohmura, Masato Yoshino, Norikazu Osada, Seiji Fujiwara, Tsuneji Kameda, Kazuya

(527) Fundamentals and Applications of Adsorption and Ion Exchange

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Florida Ballroom C

Yamada

Peter I. Ravikovitch, Chair Stefano Brandani, Co-Chair

Sponsored by: Adsorption and Ion Exchange

- **12:30 Paper 527a:** Adsorption-Induced Transformations in Flexible Microporous Frameworks: Insight from Phonon Spectra Analysis
- **Filip Formalik**, Alexander Neimark, Bogdan Kuchta
- **12:50** Paper **527b**: Material Discovery By Model Guided Targeted Synthesis for Natural Gas Storage Application
- Yogesh Joshi, Joseph Falkowski, Pavel Kortunov, Robert Colby, Gerardo Majano

- 1:10 Paper 527c: On the Use of Single, Dual and Three Process Langmuir Models for Gas Mixture Components That Exhibit Different Combinations of These Processes
- **James A. Ritter**, Kyle J. Tynan, Armin D. Ebner
- 1:30 Paper 527d: Determination of Optimal Hot Purge Gas Temperature in Regenerating Thermally an Air-Drying Zeolite 13X Column By Equilibrium Theory Analysis
- Hyungwoong Ahn
- **1:50** Paper **527e**: Thermodynamic Modeling of Ion Removal Processes *Yuan Li, Chau-Chyun Chen*
- 2:10 Paper 527f: Recycling of Nimh Batteries and Recovery of Rare Earth Elements Using ETS-10 Titanosilicate — Jay Thakkar, Blaine Wissler, Nick Dudenas, Xinyang Yin, Xueyi Zhang

(528) Fundamentals of Nanoparticle Coatings and Nanocoatings on Particles

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 20 Steven R. Saunders, Chair He Jing, Co-Chair

Sponsored by: Nanoparticles

- **12:30** Paper **528a**: Particle ALD of Tungsten Nitride As a Hydrogen Environmental Barrier Coating for Nuclear Space Propulsion
- **Sarah Bull**, Theodore Champ, Chanel Hill, Robert C. O'Brien, Charles B. Musgrave, Alan W. Weimer
- **12:50 Paper 528b:** Preparation of the Core-Shell Aluminum Nanoparticle with a Magnetic Nickel Shell
- Hongbin Shi, Tao Wang
- 1:10 Paper 528c: Internal Structure of a Drying Nanoparticle-Polymer Film *Thitiporn Kaewpetch, James F. Gilchrist*
- **1:30 Paper 528d:** Nanocoating of Metals Oxides on Nanoscale Substrates in Organic Solvents
- **Ahmed Jasim**, Yangchuan Xing, Xiaoqing He, Tommi White
- 1:50 Paper 528e: Fabrication and Characterization of Superparamagnetic Hybrid Cellulose Nanocrystals (CNC)/ Iron Oxide (Fe₃O₄) Nanoparticles
- **Mohammad J. Hasan**, Frankie A. Petrie, Ashley E Johnson, Erick S. Vasquez, Esteban E. Ureña-Benavides
- **2:10 Paper 528f:** Particle Atomic Layer Deposition of Alumina for Flash Sintering Yttria-Stabilized Zirconia
- **Rebecca O'Toole**, Bola Yoon, Christopher Gump, Rishi Raj, Alan W. Weimer
- **2:30 Paper 528g:** Modifying the Photocatalytic and Dispersion Properties of $\mathrm{TiO}_2\,\mathrm{P}_{25}$ Nanoparticles By Scalable Molecular Layer Deposition
- **Damiano La Zara**, Maximilian R. Bailey, Dominik Benz, Mike J. Quayle, Staffan Folestad, J. Ruud van Ommen

(529) Graphene and Carbon Nanotubes: Characterization, Functionalization, and Dispersion

Wednesday, Nov 13, 12:30 PM
Hyatt Regency Orlando, Discovery 44
Nigel Reuel, Chair
Shohreh Hemmati, Co-Chair

Sponsored by: Carbon Nanomaterials

- **12:30 Paper 529a:** Invited Talk: Resolving Carbon Nanotube Structures By DNA
- Ming Zheng
- 1:01 Paper 529b: Thermomechanical Behavior of Nanodiamond Superstructures in Interlayer-Bonded Twisted Bilayer Graphene
- **Mengxi Chen**, Andre R. Muniz, Dimitrios Maroudas
- 1:18 Paper 529c: Multiwalled Carbon Nanotube Functionalization and Characterization: Evidence for Lactone and Ester Formation
- Zhongyao Zhang, David Flaherty
- 1:35 Paper 529d: Growth and Modification of Carbon Nanotubes By Atomic Layer Deposition of Ni and Cu for Spaceflight Instruments and Terrestrial Applications
- **Vivek Dwivedi**, Henry Degroh, Raymond A. Adomaitis, Hossein Salami, Alan Uy, Aarathi Vadapalli, Brianna Sheard
- 1:52 Paper 529e: Growth of Small Diameter Carbon Nanotubes Using High-Melting Point Transition Metal Catalyst Promoters
- **Brian Everhart**, Rahul Rao, Benji Maruyama, Placidus B. Amama
- **2:09** Paper **529f**: 3D Layer-By-Layer Electrostatic Assembly of Graphene-Noble Metal Thin Films for Energy Storage and Conversion Applications
- Mark H. Jaskot, Joshua M. Musiol, Kamil Woronowicz, Pamela L. Sheehan, Preston Haney, Harry L. Moore, F. John Burpo, **Enoch A. Nagelli**
- 2:26 Paper 529g: Graphene Oxide-Polysulfone Mixed Matrix Membranes: Effect of Graphene Functionalization and Loading on Oil-Water Separation Performance and Membrane Fouling
- Omnya Abdalla, Ahmed Abdala
- **2:43 Paper 529h:** Mechanical Behavior of Graphene Nanomeshes
- Mengxi Chen, Augusto M. Christmann, Andre R. Muniz, Ashwin Ramasubramaniam, Dimitrios Maroudas

(530) Heterogeneous Catalysis in Liquid Media II

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Florida Ballroom A Nirala Singh, Chair Jithin John Varghese, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 530a:** Understanding and Controlling Catalytic Chemistry in the Crowded Environment of Zeolites in Liquid Phase
- Johannes A. Lercher
- 1:00 Paper 530b: Influence of Oxidant Chemical Functionality on Alkene Epoxidation over Lewis Acid Zeolites: Intermediate Stabilization through Innerand Outer-Sphere Interactions
- **Daniel T. Bregante**, Rebecca Schultz, Jun Tan, Chris Torres, Zeynep Ayla, David Flaherty
- **1:18 Paper 530c:** Controlling Selectivity in Complex Fluids with Catalytic Janus Particles
- Benjamin Greydanus
- **1:36** Paper 530d: Effects of Hydrophilic Binding Site Density in Lewis Acid Zeolites on Glucose Isomerization Catalysis
- **Juan Carlos Vega-Vila**, Michael J. Cordon, Rajamani Gounder
- **1:54** Paper 530e: Understanding and Controlling Active Sites and Their Environments for Catalysis in the Liquid Phase
- Matthew Neurock
- 2:24 Paper 530f: Theoretical Study of How Water Affects Acetic Acid Decomposition Using Density Functional Theory
- Kingsley Chukwu, Liney Arnadottir
- 2:42 Paper 530g: Heterogeneous Catalyst Stability during Hydrodenitrogenation in Supercritical Water
- **Jennifer Jocz**, Levi T. Thompson, Phillip E. Savage

(531) Highly Selective Separations with Membranes II

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Barrel Spring I Dibakar Bhattacharyya, Co-Chair Christine Duval, Co-Chair Stephen Ritchie, Co-Chair

Sponsored by: Membrane-Based Separations

- **12:30** Paper **531a**: Spiral-Wound Module with Facilitated Transport Membrane for CO₂ Capture from Flue
- **Kai Chen**, Witopo Salim, Yang Han, Dongzhu Wu, W.S. Winston Ho
- **12:51 Paper 531b:** Highly Selective Holey Graphene Oxide Membranes for Gas Separation
- **Liang Huang**, Haiqing Lin
- 1:12 Paper 531c: Hydrogen-Bonded Polyimide/Metal-Organic Framework Hybrid Membranes for Ultra-Fast Separations of Multiple Gas Pairs
- Canghai Ma, Jeffrey J. Urban
- **1:33 Paper 531d:** Enhancing H₂-Permselectivity of High-Flux Hollow Fiber Membrane Via in-Situ Layer-By-Layer Surface Treatment
- **Naveen K. Mishra**, Jaime C. Grunlan, Benjamin Wilhite

- 1:54 Paper 531e: Polymer Gas Separation Membranes Containing High Free Volume Elements and Ionic Liquids — Jason E. Bara, Irshad Kammakakam, Kathryn E. O'Harra, Grayson P. Dennis
- 2:15 Paper 531f: Ultra-Permeable and Selective Crosslinked Polymer Membranes for Energy Efficient Gas Separation
- Si Li, Gregory Kline, Ruilan Guo
- 2:36 Paper 531g: Vapor Phase Infiltration of Metal Oxides into Nanoporous Polymers for Solvent Stable Nanofiltration Membranes
- **Fengyi Zhang**, Emily McGuinness, Yao Ma, Mark D. Losego, Ryan Lively

(532) In Honor of Anthony Dixon's 65th Birthday (Invited Talks)

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Florida Ballroom B

Andrew R Teixeira, Chair N. Aaron Deskins, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 532a:** Coupled Trapping and Reaction for Emission Control of Diesel and Natural Gas Fueled Vehicles
- Michael Harold

 12:50 Paper 532b: Can Deep Neural
 Networks Make Large-Scale Resolved
- Particle CFD a Reality?

 Behnam Partopour
- **1:10** Paper **532c**: Carbon Capture *Jennifer Wilcox*
- **1:30 Paper 532d:** Some Applications and Challenges for Particle Resolved Simulation in Packed Bed Reactors
- David West
- **1:50** Paper **532e**: Identifying Diffusional Limitations during Solid Phase Peptide Synthesis in Swollen Polymer Fixed Beds
- Andrew R Teixeira
- **2:10** Paper **532f**: Layer Resolved CFD Modelling of Coated Catalyst Systems Model Validation
- **E. Hugh Stitt**, Li Liu, Sam Wilkinson, Robert Gallen, Andrew P.E. York
- **2:30 Paper 532g:** Particle-Resolved CFD in Fixed Beds Simulation or Modeling?
- Anthony G. Dixon
- 2:50 Concluding Remarks

(533) Integrated Design for Solid Drug Products

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 8 Salvador García-Muñoz, Chair Yuesheng Ye, Co-Chair Jacob Albrecht, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- 12:30 Paper 533a: Pharmaceutical Process Modeling: Mechanistic Insights of the Impacts of Roller Compaction Process Variables and Material Properties on Product Attributes
- **Hossein Amini**, Ilgaz Akseli
- **12:51** Paper **533b**: System Model for Semi-Continuous Wet Granulation Pharmaceutical Tablet Manufacturing Process
- **Boung Wook Lee**, Robert E. Yule, Christos Panos
- 1:12 Paper 533c: Assessing Performance of a Rotary Tablet Press Feeder Using the Discrete Element Method
- William R. Ketterhagen, Jeffery Larson
- **1:33** Paper **533d:** Modeling Two-Dimensional Moisture Content and Size Evolution of Pharmaceutical Granules in a Semicontinuous Fluid Bed Dryer
- Michael Ghijs, Thomas De Beer, Ingmar Nopens
- **1:54 Paper 533e:** Cracking in Drying Films of Polymer Solutions
- **Mahesh S. Tirumkudulu**, Bhawana S Tomar
- 2:15 Paper 533f: Mechanistic Mass Transport Modeling of Ionizable Drug Dissolution Under *In Vivo*-Relevant Buffer and Hydrodynamical Conditions
- **Niloufar Salehi**, Jozef Al-Gousous, Gordon Amidon, Gregory Amidon, Robert M. Ziff
- 2:36 Paper 533g: Sticking Tendency Prediction of Pharmaceutical Powders — *Ilgaz Akseli*, Chris MacTaggart, Catherine Guarino, Jianmin Li

(534) Interfacial Phenomena in Non-Aqueous Liquids

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom J Kenneth Mineart, Chair James W. Schneider, Co-Chair

Sponsored by: Interfacial Phenomena

- **12:30 Paper 534a:** Nanometer-Thick Fluorinated Ionic Liquids (ILs) As Media Lubricants in Hard Disk Drives
- **Bingchen Wang**, Catherine Moran, Lei Li
- 12:45 Paper 534b: Complete Surface Tension Characterization of Fluorinated Alcohols and Their Mixtures with Hydrogenated Alcohols: Experimental, Soft-SAFT-Dgt Modeling and MD Simulations
- José Justino, Gonçalo M. C. Silva, Pedro Morgado, Luis M.C. Pereira, Lourdes F. Vega, **Eduardo Filipe**
- **1:00 Paper 534c:** Determination of the Zeta Potential of Planar Solids in Nonpolar Liquids
- James W. Schneider, Keyi Xu, Aditya S. Khair, Dennis C. Prieve, Paul J. Sides

- **1:15** Paper 534d: Atomistic Simulations of Carbon Nanotube Deposition on Functionalized Silica Substrates
- **Zhizhang Shen**, Jonathan Dwyer, Padma Gopalan, Reid C. Van Lehn
- **1:30 Paper 534e:** QCM-D Study of the Solvent-Polymer-Catalyst Particle Interface in Fuel-Cell Inks
- **Sarah A. Berlinger**, Clayton J. Radke, Bryan D. McCloskey, Adam Weber
- **1:45 Paper 534f:** Asphaltene Adsorption from Toluene Onto Silica through Thin Water Layers
- Clayton J. Radke, Jason Hu
- **2:00 Paper 534g:** Self-Assembly and Charging of Biomimetic Surfactants in Nonpolar Solvents
- **James W. Schneider**, Keyi Xu, Paul J. Sides, Dennis C. Prieve
- 2:15 Paper 534h: Tribological Behaviors of Ionic Liquids Nanoconfined between Hydrophilic and Hydrophobic Surfaces
- **Rundong Huang**, Yuanzhong Zhang, Younjin Min
- 2:30 Paper 534i: Evidence for Self-Assembly of Tetra-Alkyl-Phosphonium 2-Cyano-Pyrrolide Ionic Liquids + Triethanolamine, Glycerol and Ethylene Glycol Systems
- Oscar Nordness, Joan F. Brennecke

(535) Interfacial Transport Phenomena

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom K Christopher L. Wirth, Chair Siamak Nejati, Co-Chair Jeffrey A. Fagan, Co-Chair

Sponsored by: Interfacial Phenomena

- **12:30 Paper 535a:** Roadway Deicing: A Pinch of Salt
- **Rukmava Chatterjee**, Daniel Beysens, Sushant Anand
- **12:45** Paper **535b:** Chaotic Thermal Convection in Micro-Scale Hydrothermal Pores Mediates Assembly of Protocell-like Vesicles
- Vijay Ravisankar, Victor M. Ugaz
- **1:00** Paper 535c: Dissolution at the Pore Scale: Comparing Simulations and Experiments
- **Anthony J.C. Ladd**, Vitaliy Starchenko, Filip Dutka, Piotr Szymczak
- **1:15** Paper 535d: Marangoni Phenomena during Droplet Formation in Microfluidics
- **Ioannis Kiratzis**, Nina M. Kovalchuk, Mark Simmons, Daniele Vigolo
- 1:30 Paper 535e: Kinetics of Phospholipid Transport to Fluid Interfaces in an Aqueous Dispersion or Laponite Gel
- **Jennifer Staton**, Stephanie R. Dungan, Laurence Talini

- 1:45 Paper 535f: Experimental and Numerical Simulation of Rayleigh-Taylor Convection with Interfacial Mass Transfer Enhancement
- **Zhen Zhang**, Qiang Fu, Xigang Yuan
- **2:00 Paper 535g:** Microgel-Covered Drops: Effects on Mass Transfer and Fluid Dynamics
- Miriam Faulde, Andreas Jupke
- 2:15 Paper 535h: Two Experimental Protocols for Accurate Measurement of Gas Component Uptake and Production Rates in Bioconversion Processes
- Kyle Stone, Q. Peter He, Jin Wang
- **2:30** Paper 535i: Experimental Study on Rayleigh-Bénard-Marangoni Convection Induced By Mass Transfer through Liquid-Liquid Interface
- **Jun Chen**, Cheng Yu, Chaoqun Shen, Zilong Deng, Xiangdong Liu

(536) Nanofabrication and Nanoscale Processing I

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Discovery 45 Jung-Sheng Wu, Chair Erick S. Vasquez, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

- **12:30 Paper 536a:** Continuous Green Millifluidic Synthesis of Ag Nanostructures
- Sina Kaabipour, **Shohreh Hemmati**
- 1:00 Paper 536b: Green Synthesis of Palladium Nanomaterials Via Biological Templates Using Tmv and Bsmv Viruslike Particles with Enhanced Stability and Customized Dimensions
- **Yu-Hsuan Lee**, Kok Zhi Lee, Corren A Scott, Rachel G Susler, Kevin V Solomon, Sue Loesch-Fries, Michael T Harris
- **1:15** Paper **536**c: Scalable Biomineralization of CdS Quantum Dots By Immobilized Cystathionine γ-Lyase *Nur Ozdemir, Joseph Cline, Christopher Kiely, Steven McIntosh, Mark A. Snyder*
- **1:30** Paper 536d: Nanoporous Aluminum Oxide Templates of Arbitrary Thickness on Silicon Carrier Wafer
- **Gibson Scisco**, Anna P. Skinner, Justin J. Hill, Kevin S. Jones, Kirk J. Ziegler
- 1:45 Paper 536e: Large-Scale Fabrication of 50nm Nanopore Array in Teflon Using Reactive Ion Etching Technique with Anodized Aluminum Oxide Templates As Etch Masks
- **Sarathy Kannan Gopalakrishnan**, Matthias A. Trujillo, Jiarang Liu, Jacob N. Chung, Kirk J. Ziegler
- 2:00 Paper 536f: Jet-Mixing Microreactor for Metal and Metal-Oxide Nanomaterial Synthesis and Scale-up Considerations
- **Pinaki Ranadive**, Aamena Parulkar, Nicholas Brunelli

2:15 Paper 536g: Synthesis of Nanostructured Cobalt Oxide Rods from Waste Lithium-Ion Batteries — Ankit Verma, Grant Johnson, Rajkumar Kore, David R. Corbin, Mark

B. Shiflett

- 2:30 Paper 536h: Continuous-Flow Microwave Synthesis of Titania Nanotubes for Moisture Harvesting — Yingjian Luo, Ana Serrano Lotina, King Lun Yeung, Miguel A. Bañares
- 2:45 Paper 536i: A Starch-Mediated Synthesis of Bimetallic Silver/Gold Nanoparticles with Different Chemical Composition As Antimicrobial and Anticancer Agents
- **David Medina**, Jorge Luis Cholula Diaz, Alfonso Nieto-Argüello, Thomas J. Webster

(537) Nanomaterials for Energy Storage II: Supercapacitors Wednesday, Nov 13, 12:30 PM

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Discovery 46

Sponsored by: Nanomaterials for Energy Applications

- **12:30 Paper 537a:** First-Principles Density Functional Theory Modeling and Machine Learning Approach for Redox Potential of Carbon Materials
- Seung Soon Jang
- **1:00** Paper **537b**: 3- D Nanostructures for Next Generation Supercapacitor Application
- Abdulsattar Alsaedi
- **1:15** Paper 537c: Se-Nanorods Decorated N-Rgonanocomposite for Application in Supercapacitors Zafar Ghouri, Ahmed Abdala
- **1:30 Paper 537d:** HTL Derived Biochar as Electrode Material for Supercapacitors
- Vinod S. Amar, Joseph Houck, Rajesh Shende
- 1:45 Paper 537e: Charge Storage Mechanism of Iron Oxide Electrode Material for Aqueous Electrochemical Energy Storage
- **Fenghua Guo**, Tongxin Zhou, Daniel S. Charles, Xiaowei Teng
- **2:00 Paper 537f:** Facile Synthesis of Porous ZnCo₂O₄@Carbon Nanofibers As Electrode for Lithium Ion Capacitors
- **2:15 Paper 537g:** Energy Dense Electrochemical Capacitors Via Advanced Nanomanufacturing and Designer Electrolytes
- **Anna P. Skinne**r, Gibson Scisco, Katherine Thomas, Kirk J. Ziegler, Kevin S. Jones, Philip Cox, Justin J. Hill
- **2:30 Paper 537h:** Potassium Sodium Niobate Based Combined Mode Piezo-Tribo Hybrid Nanogenerator
- Abu Musa Abdullah, Aminur Rashid Chowdhury, M. Jasim Uddin

- 2:45 Paper 537i: Data-Driven Tuning of Silicon Alloy Nanomaterials Properties: Novel Insights from Theory and Experiments
- **Yeseul Choi**, Anjitha S. Geetha, Christian Martin, Guro M. Wyller, Thomas J. Preston, Andrew J Adamczyk

(538) New Methods and Developments in Computational Catalysis II

Wednesday, Nov 13, 12:30 PM
Hyatt Regency Orlando, Plaza
International Ballroom F
Shaama Mallikarjun Sharada, Chair
Eric Walker, Co-Chair
Michail Stamatakis, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30** Paper **538a**: Single-NN: A Modified Behler-Parinello Neural Network with a Single Neural Network *Mingjie Liu, John R. Kitchin*
- **12:48** Paper **538b**: Reactive Force Field Derived from First Principles *Alexander V. Mironenko*, *Gregory A. Voth*
- 1:06 Paper 538c: Free Energies Calculations of CH₃OH-Pt(111) Under Liquid Solvent: DFT Force Field — Paul Meza-Morales, Rachel B. Getman
- 1:24 Paper 538d: Linked-List Based Queuing System for Kinetic Monte Carlo Simulations of Heterogeneous Catalysts — Giannis D. Savva, Michail Stamatakis
- 1:42 Paper 538e: Developing a Fingerprinting and Machine Learning Framework Linking Structural Disorder to Oxidation Behavior in Metal Grain Boundaries for CO₂ Electrocatalysis

 Matthew Curnan, Wissam A. Saidi, Judith Yang, Jeong Woo Han
- **2:00** Paper 538f: An Efficient Method for Predicting Adsorption Energies and Catalytic Performance
- Matthew Montemore
- 2:18 Paper 538g: Automated DFT Calculations for the High-Throughput Screening of Oxygen Evolution Reaction Catalysts
- **Seoin Back**, Kevin Tran, Zachary Ulissi
- 2:36 Paper 538h: Investigation of Metal Adsorption Trends on Modified MgO Supports Using Density Functional Theory and Statistical Learning — Chun-Yen Liu, Shijia Zhang, Meng Li, Thomas P. Senftle

(539) Outreach Activities for K-14: Engaging our Pipeline

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 22 Anthony Butterfield, Chair Kristine Horvat, Co-Chair Anju Gupta, Co-Chair

Sponsored by: Education

- 12:30 Paper 539a: Dual-Enrollment Introduction to Engineering with Chemical & Petroleum Engineering Applications--Course Delivery through Distance Education
- Bill B. Elmore
- **12:47 Paper 539b:** K-12 Outreach: An Emphasis on Communication
- Taryn Bayles
- 1:04 Paper 539c: Increasing Chemical Engineering K-14 Outreach By Tackling Water Conservation Using Human-Centered Design
- Anays Hernandez, Sindia Rivera-Jimenez
- **1:21** Paper **539d:** Increasing STEM Understanding and Engagement through Engineering Learning Activities *Kristine Horvat*, *Reah Thomas-Hill, Judy Randi*
- 1:38 Paper 539e: Aiche's K-12 Outreach STEM Module Competition: Results from the First Event and Future Plans
- Lucas J. Landherr
- 1:55 Paper 539f: Strategies for the Promotion of K-12 Science Education for Impacted, Multicultural Student Populations
- **Sophia M. Roberts**, Kenneth L. Roberts
- 2:12 Paper 539g: Outreach Methods and Modules in Partnership with a Geothermal Research Program
- **Anthony Butterfield**, Andrew Simonson
- 2:29 Paper 539h: How to Organize and Implement an Outreach Day to Excite, Engage, and Educate Middle School Students about Engineering Adam T. Melvin, Adrienne Steele
- 2:46 Paper 539i: Engaging Middle and High School Students in Hypothesis Generation Using a Citizen-Scientist Network of Air Quality Sensors
- Jimmy Moore, Wei Xing, Matthew Dailey, Katrina Le, Tom Becnel, Pascal Goffin, Miriah Meyer, Pierre-Emmanuel Gaillardon, Ross Whitaker, Jason Wiese, Anthony Butterfield, **Kerry Kelly**

(540) Particle Technology Awards Lectures (Invited Talks)

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 19 Bruce D. Hook, Chair James F. Gilchrist, Co-Chair

Sponsored by: Particle Technology Forum

12:30 Paper 540a: Shell Thomas Baron Award Lecture

1:10 Paper 540b: Elsevier PTF Lifetime Award Lecture

1:50 Paper 540c: PSRI Fluidization Award Lecture

Lecture

(541) Particulate and Multiphase Flows: Emulsions and Droplets

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom L

Christopher L. Wirth, Co-Chair Javen Weston, Co-Chair Ya-Wen Chang, Co-Chair Charles E. Sing, Co-Chair

Sponsored by: Fluid Mechanics

- **12:30** Paper **541a**: Probing Droplet Shape Relaxation and Its Dependence on Viscosity Using a Microfluidic Hydrodynamic Trap
- **Shweta Narayan**, Davis B. Moravec, Daryl Quam, Andrew J. Dallas, Cari S. Dutcher
- **12:45** Paper **541b**: Using Electric Fields to Manipulate Surfactant Transport to Oil-Water Interfaces
- **Rajarshi Sengupta**, Aditya S. Khair, Lynn M. Walker
- **1:00 Paper 541c:** A Continuous Approach to Synthesize Nanoemulsions Via Condensation
- Hassan Bararnia, Sushant Anand
- **1:15 Paper 541d:** Drop Production in Yield-Stress Fluids
- **Ya-Wen Chang**, Hugo Minière, Juan Reimondo, Josefa Guerrero-Millan
- 1:30 Paper 541e: Flow and Drop Breakup in a Highly Concentrated Emulsion Squeezing through a Narrow Constriction
- **Alexander Z. Zinchenko**, Robert H. Davis
- 1:45 Paper 541f: Influence of Surfactant-Nanoparticle Interactions on the Stability and Rheology of Emulsions — Ashwin Kumar Yegya Raman, Clint P. Aichele
- **2:00 Paper 541g:** Drop Deformation and Spreading in Merger of an Oil Drop with an Immiscible Liquid Pool
- **Suhas Tamvada**, Varun Kulkarni, Venkata Yashasvi Lolla, Nikhil Shirdade, Sushant Anand
- 2:15 Paper 541h: Drop Breakage in a Pump-Mixer: The Influence of Interfacial Tension and Dispersed-Phase Viscosity Han Zhou, Shan Jing, Shaowei Li
- **2:30 Paper 541i:** Flow Regimes in a T-Junction Micro-Channel Using Lattice Boltzmann Method
- Shambhu Anil
- 2:45 Paper 541j: Mesoscale Modeling of Emulsification in Rotor-Stator Devices Xiaoping Guan, Chao Chen, Ning Yang

(542) Photochemical Reaction Engineering in Fine Chemical and Pharmaceutical Industries

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom E Eric G. Moschetta, Chair Marimuthu Andiappan, Co-Chair Jonathan P. McMullen, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30** Paper **542a**: Cuprous Oxide Nanoparticles As Efficient Heterogeneous Photocatalyst for C-C Coupling Reactions
- **Ravi Teja Addanki Tirumala**, Marimuthu Andiappan
- **12:55 Paper 542b:** First-Principles Modeling of Hot-Carrier-Assisted Hydrogenation Reactions
 Tong Mou, Bin Wang
- 1:20 Paper 542c: Visible Light Driven Anti-Markovnikov Hydration of Styrene to 2-Phenylethanol in Continuous Flow Microreactor
- **Yuhang Chen**, Zhiyong Tang, Jie Zhang, Yuhan Sun
- **1:45** Paper **542d:** Using Data-Rich Experimentation to Maximize Productivity of Photochemical Reactions upon Scale-up
- **Karthik Narsimhan**, Francois Levesque, Michael Di Maso, John R. Naber, Jonathan P. McMullen
- 2:10 Paper 542e: Development of a Continuous Stirred-Tank Reactor (CSTR) Platform for Handling Heterogeneous Visible-Light Photoredox Reactions
- Alexander Pomberger, Yiming Mo, Kakasaheb Nandiwale, Rohit Duvadie, Richard I. Robinson, Klavs F. Jensen
- **2:35** Paper **542f**: A Systematic Approach to the Design and Scale-up of Photochemical Reactors
- **Melda Sezen-Edmonds**, Jose E. Tabora, Benjamin M. Cohen

(543) Polymer Thin Films, Nanoconfinement, and Interfaces I Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 11 Christian W. Pester, Chair Laura Bradley, Co-Chair

Sponsored by: Polymers

- **12:30 Paper 543a:** Understanding the Mechanism of Solvent-Driven Infiltration of Polymer (SIP) into Nanoparticle Packings
- **Neha Manohar**, R. Bharath Venkatesh, Robert A. Riggleman, Kathleen J. Stebe, Daeyeon Lee
- **12:45** Paper **543**b: Tg and Structural Recovery of Polystyrene Nanorods

 Madhusudhan Pallaka, *Sindee L. Simon*
- 1:00 Paper 543c: The Effect of Crystallization and Glass Transition Temperature in Thin Poly(D,L-lactic acid) Copolymer Films for Controlling Osteoblast Recruitment and Adhesion — Ufuoma Ikoba, Nathan Gallant, Ryan Toomey
- **1:15** Paper **543d:** Dynamic Phase Transitions in Confined Polymer Glasses *Robert A. Riggleman*
- 1:45 Paper 543e: Effect of Molecular Structure and Crosslink Density of Surface-Anchored Poly(N-alkylacrylamide) Hydrogels on Adsorption of Fibrinogen
- **Pandiyarajan Chinnayan Kannan**, Jan Genzer

- 2:00 Paper 543f: Probing the Interface of Irreversible Adsorption in Polymer Nanocomposites
- Katelyn Randazzo, Biao Zuo, Rodney D. Priestley
- 2:15 Paper 543g: Lattice Self-Consistent Field Calculations of Ring **Polymer Brushes**
- Wenjuan Qiu, Baohui Li**, Qiang** (David) Wang
- 2:30 Paper 543h: Align Graphene Layers Using Polymer Interfacial Interactions
- Weiheng Xu, Rahul Franklin, Sayli Jambhulkar, Dharneedar Ravichandran, Kenan Song
- 2:45 Paper 543i: Composites Biointerfaces for an in Vitro cellular Study
- Valentina Dinca

(544) Practical Applications of **Computational Chemistry and Molecular Simulation I**

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Rock Spring I/II Phillip R. Westmoreland, Chair Jonathan Moore, Co-Chair Joseph Golab, Co-Chair Martin Sanborn, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

- **12:30** Break
- 12:45 Paper 544b: Computationally Aided Design of Two-Dimensional Composites As Alternatives to Metallic Copper for Catalyzing the Carbon Dioxide Reduction Reaction
- **Zhou Lin**, Kun Jiang, Alejandro J. Garza, Alexis T. Bell, Martin Head-Gordon
- 1:00 Paper 544c: Tuning the Selectivity of Ethyl Disproportionation on Pt-Doped Cu(111) Surfaces: Do You Want Ethane or Ethylene?
- Romain Reocreux, Paul Kress, E. Charles H. Sykes, Michail Stamatakis
- 1:15 Paper 544d: Atomistic Simulation of Defect Formation for Quantum Information Science Applications
- Elizabeth M. Y. Lee, Giulia Galli, Juan de Pablo
- 1:30 Paper 544e: Modeling the Sintering and Redispersion of Supported Nanoparticles By Atomistic Simulations
- 1:45 Paper 544f: Sticking Efficiency of Silica Clusters By Molecular Dynamics - Eirini Goudeli, Christopher J. Hogan Jr.
- 2:00 Paper 544g: Soot Particle Structure: Insights from Molecular Dynamics and Monte Carlo Simulations - Kimberly Bowal, Jacob W Martin. Peter Grancic, Markus Kraft
- 2:15 Paper 544h: Predicting Structure and Vitrification in Toughened Epoxy Thermosets with Million-Particle Molecular Dynamics
- Eric Jankowski

- 2:30 Paper 544i: Molecular Dynamics Simulations of Zwitterionic Peptide Self-Assembly
- Dilnoza Amirkulova, Andrew White
- 2:45 Paper 544j: A Computational Study on Ionic Liquid Cation-Cytochrome P-450 Complexes Using QM/MM Calculations to Provide Structural Insights into Their Binding
- Atiya Banerjee, Jindal K. Shah

(545) Process Intensification By **Enhanced Heat and Mass Transfer**

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 17 Kishori T. Deshpande, Chair Robert Broekhuis, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

- 12:30 Paper 545a: Process Intensification Using Annular Centrifugal Extractor for Highly Exothermic Multiphase Di-Nitration Reaction - Mrityunjay Sharma, Amol Kulkarni
- 12:55 Break
- 1:20 Paper 545c: Design and Optimization of 3D Reactor Technologies for the Production of Light Olefins
- Jens N. Dedeyne, Marco Virgilio, Tony Arts, Guy B. Marin, Kevin M. Van Geem
- 1:45 Paper 545d: Control of Reactive Distillation Columns Separating Reacting Mixtures with Somewhat Unfavorable Relative Volatilities
- Shuwei Yin, Haisheng Chen, Kejin Huang, Xing Qian, Yang Yuan, Liang Zhang, Shaofeng Wang
- 2:10 Paper 545e: Intensified Liquid-Liquid Extractions for Nuclear Fuel Reprocessing – Hydrodynamics, Mass Transfer and Scale-up
- Eduardo Garciadiego Ortega, **Dimitrios Tsaoulidis**, Panagiota Angeli
- 2:35 Paper 545f: Intensification of Cephalexin Synthesis in Modular Microfluidic Devices Using Electric Field Lucie Vobecka, Alexandr Romanov, Linda Ticha, Jakub Tucek, Zdenek Slouka, Michal Pribyl

(546) Process Monitoring & Fault **Detection**

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 26 Ravendra Singh, Chair **Ankur Kumar, Co-Chair**

Sponsored by: Data and Information Systems

- 12:30 Paper 546a: Constrained Variable Selection for Distributed **Multivariate Statistical Process** Monitoring
- Shaaz Khatib, Prodromos Daoutidis
- 12:49 Paper 546b: Application of Sequential Monte Carlo Methods for Robust Monitoring of Lactic Acid Bacteria Fermentation
- **Ergys Pahija**, Robert Spann, Gürkan Sin

- 1:08 Paper 546c: Performance-Based Accommodation of Sensor Faults in Output Feedback Sampled-Data Control Systems with Measurement Delays — James Allen, Nael H. El-Farra
- 1:27 Paper 546d: A Hybrid Modeling Approach for Fault Detection and Isolation of HVAC Systems
- **Hesam Hassanpour**, Prashant Mhaskar, John M. House, Timothy I. Salshury
- 1:46 Paper 546e: Fault Detection for Pressure Swing Adsorption Processes - Jangwon Lee, Ankur Kumar, Jesus Flores-Cerrillo, Jin Wang, Q. Peter He
- 2:05 Paper 546f: Sensor and Test Selection for Passive & Active Fault Diagnosis
- **Utsav Awasthi**, Kyle A. Palmer, George M. Bollas
- 2:24 Paper 546g: Application of Chemometric Methods to Generate Reaction Pathway Hypotheses for the Thermal Cracking of Athabasca Bitumen Kaushik Sivaramakrishnan, Anjana Puliyanda, Arno De Klerk, Vinay Prasad
- 2:43 Paper 546h: Systematic Analysis, Diagnosis and Optimal Operation of an Industrial Hydrogenation System — Lingyu Zhu, Orakotch Padungwatanaroj, Yodsathorn Chavewanmas, Anjan Tula, Han Gong,

(547) Properties and Phase Equilibria for Fuels and Petrochemicals II

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Challenger 38/39

Paul M. Mathias, Chair M. R. Riazi, Co-Chair

Xi Chen, Rafiqul Gani

Sponsored by: Fuels and Petrochemicals Division

- 12:30 Paper 547a: A Comparative Review of Thermophysical Properties and Characteristics of Biofuels and Petrofuels - M. R. Riazi
- 12:55 Paper 547b: Prediction of Multicomponent Gas Adsorption Equilibria and Heat of Adsorption from Pure Component Isotherms with Adsorption NRTL Model - Hla Tun, Chau-Chyun Chen
- 1:20 Paper 547c: Development of Robust Models for the Prediction of Reid Vapor Pressure (RVP) in Fuel Blends and Their Application to Oxygenated Fuels
- Alexander Landera, Niall Mac Dowell, Anthe George
- 1:45 Paper 547d: The Effect of Bio-Derived Additives on Fatty Acid Methyl Esters for Improved Biodiesel Cold Flow **Properties**
- Michael Senra, Lindsay Soh, Stephanie McCartney
- 2:10 Paper 547e: Crude Oil Compositional Analysis Methods and Their Impact on Thermophysical Properties
- Joseph W. Hogge, David L. Lord, Raymond Allen, David K. Rudeen

- 2:35 Paper 547f: Quaternary Phase Equilibrium Data of Quaternary Water + (Ethanol and 2-Propanol) + Isooctane System
- Danielle L. de Klerk, Cara E. **Schwarz**

(548) Protein Science and **Engineering: Advances on Engineering the Physiochemical Properties of Proteins**

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 3 James A. Van Deventer, Co-Chair Joseph Rollin, Co-Chair **Shelby Brooks, Co-Chair**

Sponsored by: Bioengineering

- 12:30 Paper 548a: Molecular Sieving on the Surface of Nano-Armored Protein - Bibifatima Kaupbayeva, Hironobu Murata, Amber Lucas, Krzysztof Matyjaszewski, Jonathan Minden, Alan
- 12:48 Paper 548b: Oligomericity Is an Important Indicator in the Kinetic Stability of Biocatalytic Proteins — Adam A. Caparco, Bettina Bommarius, Robert D. Franklin, Julie A. Champion, Andreas S. Bommarius
- 1:06 Paper 548c: A Novel Technique to Characterise the Surface Hydrophobicity of Proteins Using Inverse Liquid Chromatography
- Dilip Sethi, Daryl Williams, Sarah Hedberg
- 1:24 Paper 548d: Molecular Mechanisms of Membrane Curvature Sensing By Disordered Proteins - Wade F. Zeno, Jeanne C. Stachowiak
- 1:42 Paper 548e: Discovery of Thermostable Cellobiohydrolase from Mesophilic Marine Aspergillus Niger - Li-Nian Cai, Lv Li, Dong-Qiang Lin, Shan-Jing Yao
- 2:00 Paper 548f: Using Machine Learning to Guide Protein Engineering for Biocatalysis
- Xi Han, Xiaonan Wang, Kang Zhou
- 2:18 Paper 548g: Chemogenetic Control of Organisms Using Redesigned **Proteins**
- Tim Whitehead

(549) Systems and Quantitative **Biology: Signaling Pathways, Response Networks and Growth** Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 2 Laura Jarboe, Co-Chair John Blazeck, Co-Chair Adriana San-Miguel, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 175ag: Analysis of Fn,4--NF-Kb Signaling Response Dynamics Using a Mechanistic Model

— **Jawahar Khetan**, Dipak Barua

12:48 Paper 549b: Quantitative Scaling of Virus One-Step Growth across the Domains of Life

- Herry Jin, John Yin

- **1:06** Paper **549c:** Looking Beyond GWAS: Identifying Functional Roles of SNPs Using Metabolic Networks in *Arabidopsis* and *Populus*
- **Debolina Sarkar**, Costas Maranas
- 1:24 Paper 549d: Metabolic Modeling and Pulse Amplitude Modulation Fluorometry Elucidate the Interplay between Photosynthesis and Carbon Fixation in a Purple Non-Sulfur Bacterium
- Adil Alsiyabi, Rajib Saha
- 1:42 Paper 549e: Dynamic Transcriptomic Profiling Reveals Novel Short-Term and Long-Term Strategies to Cope with Oxygen Limitation in Scheffersomyces Stipitis
- **Matthew Hilliard**, Thomas Jeffries, Q. Peter He, Jin Wang
- 2:00 Paper 549f: Markov Process Model for Cancer Growth Elucidates Tumor Escape of Immune Surveillance and Treatment
- **Isaac Pulatov**, Adeyinka Lesi, David Rumschitzki
- 2:18 Paper 549g: Invited Talk: Systems and Quantitative Biology: Signaling Pathways, Response Networks and Growth
- Ganesh Sriram

(550) Teaching Using Desktop Learning Modules and Laboratory Activities

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 23 Monica Lamm, Chair Vincent J. Tocco Jr., Co-Chair

Sponsored by: Undergraduate Education

- **12:30 Paper 550a:** Strategies for Implementation of Desktop Learning Modules
- Negar Beheshti Pour, Derek L. Englert, Isabel Escobar, John F. Maddox, Bernard J. Van Wie**, Sarah Wilson**
- **12:48** Paper **550b**: Enhancing the Design of Low-Cost Desktop Learning Module Kits for Ease of Implementation and Adoption
- Olivia Reynolds, Kitana Kaiphanliam, Aminul Islam Khan, Negar Beheshti Pour, David B. Thiessen, Olusola Adesope, Prashanta Dutta, Bernard J. Van Wie
- **1:06 Paper 550c:** Temperature Control Lab for Dynamics and Control
- John D. Hedengren, R. Abraham Martin, **Jeffrey C. Kantor, Nigel Reuel**
- **1:24 Paper 550d:** Everyone Loves Snack! Classroom Experiments You Can Eat
- Margot A. S. Vigeant
- **1:42** Paper **550e**: Reinforcing Design of Experiments, Regression, and Optimization with Paper Helicopters *Nigel Reuel*
- 2:00 Paper 550f: A Demonstration Kit for First-Order Processes and Compartmental Models — Thomas J. Mansell

- **2:18 Paper 550g:** Optimizing National Dissemination and Use of Low-Cost Desktop Learning Modules
- Katelyn Dahlke, Bernard J. Van Wie, Jacqueline Burgher Gartner, Olusola Adesope, Prashanta Dutta, David B. Thiessen, Kitana Kaiphanliam, Aminul Islam Khan, Olivia Reynolds
- **2:36 Paper 550h:** Let's Get Pumped: A Student Hand-Pump Project Intcorporated into Fluid Mechanics
- Alex J. Bertuccio

(551) Theory, Modeling, and Simulation of Nuclear Chemical Processes II

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Discovery 43 Maximilian B. Gorensek, Chair Valmor F. de Almeida, Co-Chair

Sponsored by: Nuclear Engineering Division

- **12:30** Paper **551a:** Model of Helium Bubble Density and Growth in Tungsten from Equations of State
- **Karl D. Hammond**, Dimitrios Maroudas, Brian D. Wirth
- 12:52 Paper 551b: On the Onset of 'Fuzz' Formation in Plasma-Facing Materials. I. Surface Morphological Evolution Model
- **Dwaipayan Dasgupta**, Robert Kolasinski, Dimitrios Maroudas, Brian D. Wirth
- 1:14 Paper 551c: Helium Aggregation and Surface Morphology Near Surfaces and Grain Boundaries in Plasma-Facing Tungsten
- **Karl D. Hammond**, Zhuocen Yang, Dimitrios Maroudas, Brian D. Wirth
- 1:36 Paper 551d: On the Onset of 'Fuzz' Formation in Plasma-Facing Materials. II. Effects of Subsurface Bubble Dynamics, Temperature, and Elastic Moduli of Damaged Tungsten
- **Dwaipayan Dasgupta**, Robert Kolasinski, Sophie Blondel, Asanka Weerasinghe, Dimitrios Maroudas, Brian D. Wirth
- **1:58 Paper 551e:** Mechanisms of Rubidium and Krypton Release from Zeolite Getters
- Amir M. Mofrad, Karl D. Hammond
- **2:20 Paper 551f:** Defect Interaction Energetics and Stress State of Plasma-Exposed Tungsten
- Asanka Weerasinghe, Lin Hu, Dwaipayan Dasgupta, Karl D. Hammond, Brian D. Wirth, Dimitrios Maroudas
- **2:42** Paper **551g**: Thermomechanical Properties of Plasma-Exposed Tungsten *Asanka Weerasinghe*, *Brian D*.

Wirth, Dimitrios Maroudas

(552) Thermochemical Conversions of Lignins and Lignocellulosics

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Discovery 47 Chang Geun Yoo, Chair Justinus A. Satrio, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

- 12:30 Paper 552a: Production of Hydrocarbons from Fast Hydropyrolysis of Lignin at Atmospheric Pressure Promoted By Nickel inside Carbon-Nanotube Reactors
- Bingliang Zhou, Heather Wise, Fernando Resende, Anthony Dichiara
- 12:55 Paper 552b: Kinetic Study of Tire Carbon Black and Biomass Soot Steam Activation Used for the Removal of Phenol and Chlorine from Drinking Water
- Manuel Garcia-Perez**, Anna Trubetskaya**
- **1:20 Paper 552c:** The Effect of Wood Composition and Supercritical CO₂ Extraction on the Charcoal Production
- Anna Trubetskaya, Gerrit Ralf Surup, Fredrik Forsberg, Thomas Attard, Andrew Hunt, Vitaliy Budarin, Victor Abdelsayed, Dushyant Shekhawat
- **1:45 Paper 552d:** Lignin Hydrogenolysis with in-Situ Glycerol Aqueous Phase Reforming
- Robertus Dhimas Dhewangga Putra, Yanuar Philip Wijaya, Heather L. McKenzie-Trajano, Chang Soo Kim
- **2:10** Paper **552e**: Synthesis of Photocatalytic Hydrochars and Application of Emerging Contaminants Degradation
- **Novin Mehrabi**, Nepu Saha, M.Toufiq Reza, Nirupam Aich
- **2:35 Paper 552f:** Analysis of Pyrolysis Oil Model Compounds Using *in-Situ* Raman
- Adhish Madugula, Tracy J. Benson

(553) Thermophysical Properties: Polar Compounds and Self-Assembly Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Silver Spring I/II

Hyatt Regency Orlando, Silver Spring Erik E. Santiso, Chair Clare McCabe, Co-Chair Sanket A. Deshmukh, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **12:30** Paper 553a: Quantifying the Role of Polarizability in the Self-Organization of Ionic Liquid Crystals *Michael Quevillon, Jonathan K.*
- **Michael Quevillon**, Jonathan k Whitmer
- **12:46 Paper 553b:** Monte Carlo Simulation of Cylinders with Short-Range Attractions
- **Harold W. Hatch**, Nathan A. Mahynski, Ryan Murphy, Marco A. Blanco, Vincent K. Shen
- **1:02** Paper 553c: Molecular Modeling of Ionic Liquid-Ionic Liquid Mixtures with a Common Anion
- **Pratik Dhakal**, Jindal K. Shah

- **1:18 Paper 553d:** Self-Assembly and Phase Transition of Amphiphiles at Solid-Liquid Interfaces
- **Yao Wu**, Yingzhen Ma, Jin Gyun Lee, Lilin He, Gernot Rother, Bhuvnesh Bharti, William A. Shelton Jr.
- **1:34 Paper 553e:** Activity Coefficients of Salts in Aqueous and Nonaqueous Solvents and in Solvent Mixtures
- **Andrew Crothers**, Clayton J. Radke, John Prausnitz
- **1:50** Paper **553f**: Machine Learning for Predicting Pitzer Parameters Based on Ion Specific Properties
- **Petteri Kangas**, Risto Pajarre, Peter Blomberg, Karri Penttilä, Marja Nappa, Pertti Koukkari
- **2:06 Paper 553g:** Self-Assembly and Phase Behavior of Hyperbranched Copolymers
- **Walter G. Chapman**, Yuchong Zhang, Shun Xi
- **2:22** Paper **553h**: Discrete Modeling Approach Using Dice-like Molecules for Excess Gibbs-Energy Models
- Christoph Mayer, Thomas Wallek
- 2:38 Paper 553i: A Novel Approach to Include Double and Triple Bond Polarization in Unsaturated Hydrocarbons By Polar Solvents in an Equation of State
- Bennett D. Marshall

(554) The Use of CFD in Simulation of Multiphase Mixing Processes Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Bayhill 32 John A. Thomas, Chair Christopher Tyler, Co-Chair

Sponsored by: North American Mixing Forum

- **12:30** Break
- **12:51** Paper **554b**: Optimization of Cleaning in Process Equipment Via CFD Studies
- **Evgenii Burlutskii**, Harry E.A. Van den Akker, Orest Shardt
- 1:12 Paper 554c: Development of a CFD-DEM Model in Non-Inertial Frame for Solid-Liquid Mixing Applications Bastien Delacroix, Bruno Blais, Louis Fradette, Francois Bertrand
- **1:33 Paper 554d:** Design Optimization of Contra-Rotating, Baffle-Free Impellers for Maximizing Solid-Liquid Mixing Efficiency
- **Pongsarun Satjaritanun**, John A. Regalbuto, John R. Regalbuto, Sirivatch Shimpalee, John W. Weidner
- **1:54** Paper **554e:** Immiscible Liquid-Liquid Mixing Strategy in an Agitated Chemical Reactor – a Computational Fluid Dynamics Study
- **Rui C. Silva**, Maria Inês Lopes, Filipe Neves
- 2:15 Paper 554f: Computational Investigation of Particle Clustering in Low Reynolds Number Stirred Tanks — Weicheng Xu, Xin Feng, Steven Wang, Chao Yang

2:36 Paper 554g: Numerical Simulation of Droplet Size Distribution in Pulsed Disc and Doughnut Column with Wettable Internals

- Xiong Yu, Shan Jing, Shaowei Li

(555) Topical Plenary: Frontiers in Green Process Engineering (Invited Talks)

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Regency Ballroom Q Wei Liu, Chair Jian Liu, Co-Chair Yizu Zhu, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

12:30 Paper **555a:** CO₂ Conversion to 3D Graphene for Clean-Energy Application

— Yun Hang Hu

12:55 Paper 555b: Waste Plastics to Energy Storing Carbon Anodes through Green Processing

— Vilas G. Pol

1:20 Paper 555c: Multiscale Metabolic Modeling of the Oleaginous Microalga Chlorella vulgaris in a Photobioreactor — Juan D. Tibocha-Bonilla, Cristal Zuniga, Jared T. Broddrick, Karsten

Zengler, Rubén D. Godoy-Silva

1:45 Paper **555d**: Molecular Simulation and Experimental Study of CH₄ Adsorption in Surfactant Solution

— Yihan Xue

(556) Wide Bandgap Materials for Electronic and Photonic Applications

Wednesday, Nov 13, 12:30 PM Hyatt Regency Orlando, Celebration 15 Kevin M. McPeak, Chair Jiancheng Yang, Co-Chair

Sponsored by: Electronics and Photonics

12:30 Paper **556a:** Investigation of Process Techniques for Ga_2O_3 Based Diodes

— Fan Ren, Jiancheng Yang, Patrick Carey IV, Chaker Fares, Minghan Xian, Stephen J Pearton, Marko Tadjer

1:00 Paper 556b: Radiation Damage Effects in Ga₂O₃ Materials and Devices — Chaker Fares, Patrick Carey IV, Jiancheng Yang, Minghan Xian, Fan Ren, Jihyun Kim, Alexander Polyakov, Stephen J Pearton

1:30 Paper 556c: Radiation and Electron-Injection Induced Effects in Ga₂O₃ Schottky Rectifiers

— **Sushrut Modak**, Leonid Chernyak, Jiancheng Yang, Fan Ren, Stephen J Pearton

1:55 Paper 556d: 30 a Forward Current with 240 V Reverse Breakdown Ga₂O₃ Field-Plated Schottky Rectifiers — *Jiancheng Yang, Minghan Xian,* Patrick Carey IV, Chaker Fares, Jessica Partain, Fan Ren, Marko Tadjer, Stephen J Pearton, Akito Kuramata

2:15 Break

2:35 Paper 556f: High Dielectric Semiconductor Nanostructures with Tunable Mie Resonance in the Visible to Near-IR Region

— Farshid Mohammadparast, **Sundaram Bhardwaj Ramakrishnan**, Ravi Teja Addanki Tirumala, Marimuthu Andiappan

(557) Ammonia as a Fuel Wednesday, Nov 13, 1:45 PM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

1:45 Paper 557a: Arpa-E Refuel Program: Distributed Production of Ammonia and Its Conversion to Energy

— Grigorii Soloveichik

2:08 Paper 557b: Technical & Economic Study for Commercial Ships with HFO, LNG and NH₃ As Fuel — Hyuk Kwon, Mincheol Ryu, Su-Kyung An

2:31 Paper **557c:** High-Efficiency Two-Stroke Internal Combustion Engine

— James Ganley

2:54 Paper 557d: Our Improved Farm Tractor Ammonia and Hydrogen Fueling System

— David Toyne

3:17 Paper 557e: Fuel Transition Scenarios for the Maritime Industry up to 2050

— **Domagoj Baresic**, Tristan Smith, Carlo Raucci

(558) General Poster Session II Wednesday, Nov 13, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

Sponsored by: Poster Sessions

Paper 558a: Catalytic CO-Hydrogenation Co-Fed with Ammonia to Produce Fatty Amines and Nitriles

— Viacheslav lablokov, Norbert Kruse, **Hafsa Karroum**

Paper 558b: Precise Engineering of Oxide Supported Atomically Dispersed Rh Local Environment for Alkene Hydroformylation

— **Insoo Ro**, Gregory Zakem, Phillip Christopher

Paper 558d: Physical Descriptors for Predicting Charge Transfer at the Metal-Support Interface

— Chun-Yen Liu, Thomas P. Senftle

Paper 558e: Application of Structure Descriptor for Rational Design of Transition Metal Catalysts

— Daojian Cheng

Paper 558f: Superior Active Oxygen Transfer Ability of CuO/CeO₂ catalyst with Enhanced Activity for Preferential CO Oxidation

— Yana Xia

Paper 558g: Small Scale Production of $\rm H_2$ Via Autothermal Reforming in an Adiabatic Packed Bed Reactor

Syed Abbas, Ramesha Tariq

Paper 558h: Multiple Applications of 2D Titanium Carbide (MXene) in Photoelectrochemical Water Splitting: Cocatalysts, Surface Modifications and Matrix for Chemical Transformation

— Jikai Liu, Dejian Yan, Hui Chang, Hal

Paper 558i: In Situ Formed Pt₃Ti Nanoparticles on Two-Dimensional Transition Metal Carbide (MXene) As Efficient Catalysts for Hydrogen Evolution Reaction

- Yue Wu

Paper 558j: A Density Functional Study of Transition Metal Fischer Tropsch Catalysts

- Sumegha Godara

Paper 558k: Effective Diffusion
Coefficient of Isobutane, 2,3 DimethylButane, Hexane and Decalin in Ternary
Blends of Adsorbates (Liquid Phase):
Spent PtSOxZrTi and CeNax Catalysts
— Roberto E. Galiasso Tailleur, Rough
P Ronaldi

Paper 5581: Role of Intra-Particle Grain Boundaries in CO₂ Electroreduction — Noushin Omidvar, Soojin Jeong, Xingchen Ye, Hongliang Xin

Paper 558m: Ammoxidation of Toulene By Using V₂O₅/Al₂O₃ As Catalyst to Synthesize Benzonitrile

- Aizaz Mateen Sr.

Paper 558n: Intrinsic Reaction
Kinetics and Mechanism for the
Transesterification Reaction to Diphenyl
Carbonate Catalyzed By Dibutyltin Oxide
— Xia Yin, Yi Zeng, Jie Yao, Zhiping
Du, Zhiguo Yan, Gongying Wang

Paper 558o: The Effect of Silanol Groups on Silica-Supported Cobalt Catalysts in Fischer-Tropsch Synthesis. — Chike G. Okoye-Chine, Mahluli Moyo, Yali Yao, Xinying Liu, Diane Hildebrandt

Paper 558p: Theory of Mixed Ion-Electron Transfer Kinetics in Intercalation Electrodes

— **Dimitrios Fraggedakis**, Michael McEldrew, Martin Z. Bazant

Paper 558r: Electrolyte Engineering for Efficient Electrochemical Nitrate Reduction to Ammonia

— Joshua M. McEnaney, Sarah Blair, Adam Nielander, Jay Schwalbe, Matteo Cargnello, Thomas F. Jaramillo

Paper 558s: Production of Syngas with Controllable H₂/CO Ratio By High Temperature Co-Electrolysis of CO₂ and H₂O over Ni- and Co- Doped Lanthanum Strontium Ferrite Perovskites

— **Dhruba Jyoti Deka**, Seval Gunduz, Taylor Fitzgerald, Jeffrey T. Miller, Anne Co, Umit S. Ozkan

Paper 558t: Engineering Geometric and Defective Nanostructures of Carbon Materials for Selective Carbon Dioxide Electro-Reduction

— Jingjie Wu, Tianyu Zhang

Paper 558u: Catalysis inside Hollow Nanostructured Materials: The Balanced Adsorption-Diffusion Effect

- Yue Wang, Dawei Yao, Xinbin Ma

Paper 558v: Calculation of Catalytic Activity for Alloy Nanoparticles with Experimentally Relevant Sizes By Explicitly Predicting Adsorbate Binding Energy

- Liang Cao, Tim Mueller

Paper 558w: Using Atomic Layer Deposition to Design Catalysts for Enhanced Pairwise Selectivity of Parahydrogen Addition to Unsaturated Hydrocarbons

— Bochuan Song, **Helena Hagelin-Weaver**, Diana Choi, Clifford R. Bowers

Paper 558x: Deconvolution of Faceted Platinum Alloy Nanoparticle Catalyst Growth Pathway from in Situ Characterizations

— Xiaochen Shen, Changlin Zhang, Yanbo Pan**, Zhenmeng Peng**

Paper 558y: Enhancing Lactic Acid Production from the Dihydroxyacetone By Extra Framework Alumina

— Md. Anwar Hossain, Mohammad Shahinur Rahaman, Noppadon Sathitsuksanoh

Paper 558z: Why is PBR Better than BTR for the Kinetics Studies of Heterogeneous Catalytic Reactions? The Case of Conversion of Fructose to HMF — Juliana Tacacima, Silas Derenzo, Joao G. R. Poco

Paper 558aa: MOF-Derived Sulfur-Nitrogen-Doped Copper Nanoparticles for the Selective Electrocatalytic Reduction of $\mathrm{CO_2}$ to Formate

- Bike Zhang, Yao Shi, Yi He

Paper 558ac: Discover Perovskites for Electrocatalytic Water Oxidation Via Adaptive Machine Learning — Zheng Li, Hongliang Xin

Paper 558ad: Enhanced Alkaline Oxygen Evolution Using Hybrid Co@Ni₁₂P₅/Ppy

— Swetha Ramani, Sadik Çoğal, Jeffrey Lowe, Venkat Bhethanabotla, John Kuhn

Paper 558ae: Apparent Kinetic Rate Expressions of Light Olefins Alkylation of Isobutane Using a PtSO₄ZrTiSO/SiO₂ Meso-Structured Catalyst

— Roberto E. Galiasso Tailleur, Carlos Farina

Paper 558af: One-Step Synthesis of Cobalt Oxide Catalyst in a Flame Aerosol Reactor for Oxygen Removal from CO₂-Rich Oxy-Coal Combustion Flue Gas

- Sungyoon Jung, Pratim Biswas

Paper 558ag: Elucidating the Roles of Support and Environment on Sulfated Metal Oxides

— Justin Marlowe, George Tsilomelekis **Paper 558ah:** Dynamic Catalysis and Surface Resonance for Turnover Frequency Enhancement

— **M. Alexander Ardagh**, Omar A. Abdelrahman, Qi Zhang, Paul Dauenhauer

Paper 558ai: Lithium Dendrite Suppression with Lithiated Nafion As a Polymer Electrolyte

— **Paria Coliaie**, Aditya Prajapati, Meenesh R. Singh

Paper 558aj: Effects of Cadmium and Mercury on the Germination of Lolium Perenne

— Yuby Cruz, Jorge L. Gallego, Carolina Montoya-Ruiz, Juan F. Saldarriaga Sr.

Paper 558al: Equilibrium Solubility, Modeling and Enthalpy of CO₂ Absorption in Aqueous Blend of Methyldiethanolamine and Arginine at Low Pressure

— **Abdelbaki Benamor**, Ahmed Gomaa Talkhan, Mustafa Nasser, Muftah El-Naas, Sahar El-Marsafy, Sayed El-Tayeb

Paper 558am: Influence of 1-(2-aminoethyl)Piperazine As a Promoter on the Equilibrium CO₂ Solubility in Aqueous N-Methyldiethanolamine & 2-Amino-2-Methyl-1-Propanol Solvent System — Anirban Dey, Sukanta Kumar Dash, Bishnupada Mandal

Paper 558an: Chinese Ink Modified Stainless Steel As a High Performance Anode in a Microbial Fuel Cell

— **Haoliang Wu**, Zhongjian Li, Zipeng Ye, Yumeng Huang

Paper 558ao: Systematic Process Intensification of Refinery Processes Using Building Blocks

— **Ashwini Ravindran**, Jianping Li, Salih E. Demirel, M. M. Faruque Hasan

Paper 558ap: Utilization of the Nanosilica Synthesis Process Generated Waste in Concrete Blocks: An Environmental Friendly Solution

— **Prabhat Vashistha**, Vivek Kumar, S.K. Singh

Paper 558aq: Coupling Computational Fluid Dynamics and Detailed Process Modeling to Efficiently Design and Improve Processes

— Ravindra Aglave, **Thomas Eppinger**

Paper 558ar: The Use of Gaseous Metal Oxide As an Oxygen Carrier in Coal Chemical Looping Combustion

— **Quan Zhang**, Tomasz Wiltowski

Paper 558as: The Direct Utilization of Shrimp Shells Using Ionic Liquid-Based Solvent

— **Xingmei Lyu**, Mi Feng, Suojiang Zhang

Paper 558at: Highly Selective Electrochemical Reduction of CO₂ to Formate Via Ultrathin Nanosheet in₂S₃ in Ionic Liquid

— **Jiaqi Feng**, Hongshuai Gao, Suojiang Zhang, Xiangping Zhang Paper 558au: A Rapid and Accurate QSPR Model for NH₃ Solubility Prediction in Ionic Liquids

— **Wenhui Tu**, Shaojuan Zeng, Xiangping Zhang

Paper 558av: Ionic Liquids Confined with Mesoporous Silica for Boosting Catalytic Conversion of CO₂ into Cyclic Carbonates

— **Qian Su**, Weiguo Cheng, Suojiang Zhang

Paper 558aw: High Performance Cobalt-Based IL/PIM-1 Thin Film Composite Membrane for Air Separation — Jiuli Han, Lu Bai, Shuangjiang Luo, Xiangping Zhang

Paper 558ax: Carbon Dioxide Activation and Electroreduction in Ionic Liquids Systems

— Suojiang Zhang

Suojiang Zhang

Paper 558ay: The Size-Controlled Structure and Dynamical Property of Ionic Liquid inside the Nano-Confined Space

— **Yanlei Wang**, Chenlu Wang, Suojiang Zhang

Paper 558az: Formulation of Complex Ionic-Liquids Electrolytes for High-Voltage Nanohybrid Supercapacitors — Shanshan Pan, Haitao Zhang,

Paper 558ba: Ionic Liquid-Based Gas Separation: From Material Design to Applications

— **Xiangping Zhang**, Haifeng Dong, Shaojuan Zeng, Yi Nie

Paper 558bb: Efficient Ambient-Air-Stable HTM-Free Carbon-Based Perovskite Solar Cells

— Xia Tao, Yan-Zhen Zheng

Paper 558bc: Choline Chloride-Urea Based Deep Eutectic Solvent As Chemical and Physical Means of Hydrogen Storage

— Kyle McGaughy, M.Toufiq Reza

Paper 558bd: Biochar As an Effective Additive to Enhance Anaerobic Digestion of Easily Acidified Food Waste — Haoqin Zhou, Robert C. Brown, Zhiyou Wen

Paper 558be: Viscoelasticity and the Validity of Time-Concentration Superposition in Nanocolloidal Suspensions

— Dinesh Sundaravadivelu Devarajan, Pouria Nourian, Gregory B. McKenna, Rajesh Khare

Paper 558bf: The Aggregate Structures of Magnetic Cubic Particles in Thermodynamic Equilibrium By Means of Brownian Dynamics Simulations

— **Kazuva Okada**. Akira Satoh

Paper 558bg: High Strength 3D Aluminum Foam Current Collector for the Better Performances of the Lithium-Ion Battery and the Supercapacitor

— **Zhoufei Yang**, Weizhong Qian

Paper 558bh: A Novel Online State of Health Estimation of Li-lon Cells

— Saeed Khaleghi Rahimian, Ying Liu

Paper 558bi: First-Principles Investigation of Aluminum Intercalation and Diffusion in TiO₂ Materials: Anatase Versus Rutile

— **Weiqiang Tang**, Cheng Cai, Xiaochen Yu, Shuangliang Zhao

Paper 558bl: PIM Incorporated High Performance Blend Anion Exchange Membranes for Fuel Cell Application — Shoutao Gong, Lv Li, Panyue Li, Yabin Jia, Ruiting Zhou, Fengxiang

Paper 558bm: Effective Methods to Pre-Treat Wastewater Retentate and Reuse the Treated Wastewater Retentate on the Pressure Retarded Osmosis (PRO) Process

— **Tianshi Yang**, Chun Feng Wan, Junying Xiong, Chakravarthy S. Gudipati, Tai-Shung Chung

Paper 558bn: Pre-Treatment of Wastewater Retentate to Mitigate Fouling on the Pressure Retarded Osmosis (PRO) Process

— **Tianshi Yang**, Chun Feng Wan, Junying Xiong, Chakravarthy S. Gudipati, Tai-Shung Chung

Paper 558bo: Reaction Software Ecosystem and Data Hub for Heterogeneous Catalysis

— **Jonathan Lym**, Gerhard R. Wittreich, Udit Gupta, Bharat Medasani, Dionisios G. Vlachos

Paper 558bp: Suppressing the HER for the Electrochemical Synthesis of Ammonia By Using a Cu-Ag Bi-Metallic Catalyst.

— **Nishithan C. Kani**, Meenesh R. Singh

Paper 558bq: Integrated Carbon Capture, Utilization, and Storage for the Midcontinent United States

— **Mackenzie Scharenberg**, Andrew Duguid, Isis Fukai

Paper 558br: Effect of Impregnation Strategy on the Performance of Pt/Ceria-Zirconia Low Temperature Reforming Catalysts

— **Yetunde O. Sokefun**, Babu Joseph, John N. Kuhn

Paper 558bs: Regeneration Energy and Thermal Stability Studies of Amine-Based Deep Eutectic Solvents for Carbon Dioxide Capture

— **Inas M. Alnashef**, Idowu Adeyemi, Mohammad Abu Zahra

Paper 558bt: Study on Optimal Side Draw Amine Design to Improve the Performance of the Post-Combustion CO₂ Capture Processes

— **Yiling Xu**, Thomas Ho, Qiang Xu

Paper 558bv: Understanding Fe-Based Catalysts for Electrochemical Ammonia Synthesis at Ambient Conditions

- Lin Hu, Xiaofeng Feng

Paper 558bw: Synthesizing Crystalline Silver Selenide Nanostructured Thin Films for Thermoelectric Applications

— Nan (Louise) Chen, Ayaskanta Sahu

Paper 558bx: An Integrated Approach for Capturing and Utilizing CO₂ in Pulp and Paper Mills: Preliminary Economic Assessment of CO₂ Capture from Lime Kiln Operations

— **Amod Parkhi**, Selen Cremaschi, Zhihua Jiang

Paper 558by: Research of the Vertical Falling Film Behavior in the Scrubbing-Cooling Tube

— **Yifei Wang**, Liucheng Yan, Xin Peng, Guangsuo Yu, Fuchen Wang

Paper 558bz: Catalytic
Deoxydehydration of Glycerol to Allyl
Alcohol with 2-Hexanol As H-Donor —
Catalyst Development and Separation
Process

— Karen Silva Vargas, Benjamin Katryniok, Marcia Araque Marin, Sebastien Paul, Franck Dumeignil

Paper 558ca: Sol Gel Prepared Fe and Ni Based Catalyst for Pyrolysis-Catalysis of Waste Plastics for Hydrogen and Carbon Nanotubes

— **Dingding Yao**, Chi-Hwa Wang

Paper 558cb: Machine Learning Molecular Dynamics for Understanding Nonadiabatic Surface Reactions — *Jiamin Wang*, Hongliang Xin

Paper 558cc: Combining Experimental Kinetics and Thermodynamic Modeling with IR Spectroscopy and Machine Learning for Fundamental Studies and Fast Product Quantification

 Natalia Rodriguez Quiroz, Joshua Lansford, George Tsilomelekis, Dionisios G. Vlachos

Paper 558cd: A Droplet-Based Evaporative Crystallization System for Protein Crystallization Kinetics Estimation

— **Moo Sun Hong**, Amos E. Lu, Jaehan Bae, Jong Min Lee, Richard D. Braatz

Paper 558cf: Optimization of Reduction Cell Efficiency for UO₂ to Uranium Metal — Jarom Chamberlain, Michael F. Simpson

Paper 558cg: Growth Curve of Chitinbacter Tainanensis at Elevated Temperature

— Chao-Lin Liu, Hsiao-Yin Chan

Paper 558ch: Block Copolymer Micellization Kinetics Measured By Time-Resolved Small Angle X-Ray Scattering

— Joseph Kalkowski, **Chang Liu**, Paola Leon Plata, Magdalena Szymusiak, Pin Zhang, Thomas Irving, Ying Liu

Paper 558ci: Hydrophilic Magnetic Ionic Liquid-Based Draw Solutes in Forward Osmosis for Sea Water Desalination

— **Hana G. Zeweldi**, Anelyn Bendoy, Hanseung Kim, Eldin M. Johnson, Wook-Jin Chung, Grace M. Nisola

Paper 558ck: Thermocatalytic Splitting of CO₂ into Fuels Using Sol-gel Derived Ni-Mg-Ferrite

— Gorakshnath Takalkar, **Rahul Bhosale**, Suliman Rashid

(559) Poster Session: Advances in Fossil Energy R&D

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Dushyant Shekhawat, Chair Rameshwar D. Srivastava, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

Paper 559a: Microwave-Assisted Reactions for Fuel Conversion

— **Dushyant Shekhawat**, Mark Smith, David Berry, Victor Abdelsayed, Christina Wildfire, Candice Ellison

Paper 559b: National Energy Technology Laboratory's National Risk Assessment Partnership (NRAP): Efforts to Reduce Risk and Ensure Successful Storage — M. Kylee Underwood, Kanwal Mahajan, Traci Rodosta

Paper 559c: A Comparison of the Effectiveness of Three Types of Borehole Seismic Technologies for Monitoring CO₂ Injected into Carbonate Pinnacle Reefs

— Mark Kelley, Liviu Grindei, Thomas Coleman, Conrad Kolb, Rich van Dok, Janice Gregory-Sloan

Paper 559d: Capillary Flow of Diluted Bitumen in Constricted Micromodel

— **Kiarash Keshmiri**, Neda Nazemifard, Haibo Huang

Paper 559e: Monitoring of an Active CO₂-EOR Field Using Charged Wellbore Casing Controlled Source Electromagnetics

— **Trevor Irons**, Nathan Moodie, Andy McAliley, Richard Krahenbuhl, Benjamin R. Bloss, Yaoguo Li, Katrina Zamudio, Michael Pace

Paper 559f: MVA Lessons Learned from Ccus Project at the Farnsworth Unit, Texas

— Richard Esser, **Brian McPherson**

Paper 559g: Geologic Carbon Storage of Anthropogenic CO₂ Under the Colorado Plateau in Emery County, Utah — Nathan Moodie, Wei Jia, Richard Middleton, Sean Yaw, Si-Yong Lee, Richard Esser, Ting Xiao, David Wheatley, Peter Steele, Brian

Paper 559h: Uncertainty Analysis of Impact of Geochemical Reactions on Forecasting CO₂ Storage at a Depleted Oil Field

McPherson

Nazemifard

— Wei Jia, Ting Xiao, Nathan Moodie, **Brian McPherson**

Paper 559i: Impact of Relative Permeability and Capillary Pressure Parameters on Chemical Trapping Predictions in Ccus

— Vivek Patil, Nathan Moodie, **Brian McPherson**

Paper 559j: Total Internal Reflection Fluorescence Microscopy: Dual Color Imaging on Oil Sands Tailing Ponds — Seyedehniloufar Manafi, Neda Paper 559k: Geochemical Characterization of Shale Rocks By Laser Induced Breakdown Spectroscopy (LIBS)

— **Jinesh Jain**, Daniel Hartzler, Chet Bhatt, Dustin McIntyre

Paper 559I: Experimental Investigation of Synergy between Low Salinity and Polymer Flooding in Enhancing Heavy Oil Recovery on Alaska North Slope

— Yang Zhao, Shize Yin, Jiangiao

Paper 559m: NMR Relaxation and Diffusion in Model Organic Shale Using Molecular Simulations

Leng, Baojun Bai

— **Arjun Valiya Parambathu**, Dilip Asthagiri, Philip Singer, George J. Hirasaki, Walter G. Chapman

Paper 559n: Determination of Confined Fluid Phase Behavior Using Modified Peng-Robinson Equation of State

— **Gang Yang**, Zhaoqi Fan, Xiaoli Li

Paper 5590: Investigations on Petrophysical Property Alterations Induced By CO₂ Injection into Sandstone Reservoirs

— E.J Kutsienyo, William Ampomah, Qian Sun, Junyu You, Robert Balch, Martha Cather

Paper 559p: Optimized Immiscible CO₂ Injections for Enhancing Tight Oil Recovery

— **Kaiqiang Zhang**, Songyan Li, Na Jia

Paper 559q: Produced Water Purification By a Vacuum Flow-through Evaporation

— Ghader Mahmodi, Shailesh Dangwal**, Seok-Jhin Kim**

Paper 559r: New Nanocatalyst Preparation for Improving Product Quality of in-Situ Upgrading Technology (ISUT)

— **Milad Ahmadi Khoshooei**, Carlos Scott, Lante Carbognani, Pedro Pereira-Almao

Paper 559s: Thermodynamic Investigation of the Ca-Mg-CO₂ System — *Dale Prentice*, *Anna Stepien*,

Magdalena Balonis, Erika Callagon La Plante, Gaurav Sant, Dante Simonetti

Paper 559t: A New Computational Model to Predict Multiphase Behaviour of Brine/CO₂/Oil/Surfactant Mixtures for LSS-WACO, EOR

— Yilei Song, Zhaojie Song, Jirui Hou

Paper 559u: Regional Economic Impacts of Carbon Capture and Sequestration

— **Josh Stanislowski**, Steve Schlasner, Bruce Folkedahl, Mike Swanson, Melanie Jensen

Paper 559v: Using CO₂-Responsive Nanogel to Improve CO₂ Flooding Sweep Efficiency and CO₂ Storage Efficiency

— **Xindi Sun**, Jiaming Geng, Baojun Bai

Paper 559y: Improved Design of a Diesel-Driven Solid Oxide Fuel Cell System for Auxiliary Power Unit Applications

— **Minseok Bae**, Joongmyeon Bae, Sai P. Katikaneni Paper 559z: Hydrogen Production from Carbonaceous Feedstocks Using a Novel Solar Rotary Kiln Reactor

— **Nicolás A. Ripoll Kameid**, Mario G. Toledo Torres

Paper 559aa: Development of a Dual Fluidized Bed Reactor for Solar Thermal Storage

— Su Been Seo, Hyung Woo Kim, Seo Young Kang, Eun Sol Go, **See Hoon Lee**

Paper 559ab: Development of a High-Purity Hydrogen Production Skid Unit for Hydrogen Refueling Stations

— **Woohyun Kim**, Dong Joo Seo, Sang Ho Park, Young Jae Hwang, Wang Lai Yoon, Jin Su Kim, Eui Hyun Cho, Dong Su Ha

Paper 559ac: Hydrogen Isotope Separation By a Palladium-Based Membrane

— **Nicholas C. Means**, Bret H. Howard, Daniel J. Haynes, Dushyant Shekhawat

Paper 559ad: Adsorptive Desulfurization of Liquid Fuels at Elevated Temperatures Using Metal Exchanged Zeolite Y

— **Priscilla Dias da Silva**, Samantha Samaniego, Kyriacos Zygourakis, Michael S. Wong

Paper 559ae: Numerical Modeling on Water and Heat Recovery from Combustion Flue Gas

— **Mohammad Abutayeh**, Kwangkook Jeong, Youngmin Kim, Gyubaek Cho

(560) Poster Session: Catalysis and Reaction Engineering (CRE) Division Wednesday, Nov 13, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom R/S

Sarsani Sagar, Chair Jesse Q. Bond, Co-Chair Thomas J. Schwartz, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

Paper 560a: Reactivity of Ni-Co/γ-Al₂O₃ Catalysts for Hydrodeoxygenation of Guaiacol

— **Deepak Raikwar**, Saptarshi Majumdar, Debaprasad Shee

Paper 560b: "H₂ -Free" Hydrodeoxygenation of Guaiacol over Ni-Mo/CeO₂-C Nanocatalysts

— Wei Jin**, Laura Pastor-Perez**, Juan Jose Villora Pico, Sai Gu, Antonio Sepúlveda-Escribano, Tomás Ramirez-Reina

Paper 560c: Microwave Carbocatalysis for Bioenergy and Biochemical Conversion

— **Armando T. Quitain**, Elaine G. Mission, Tomomi Hasunuma, Jonas Karl N. Agutaya, Mitsuru Sasaki, Tetsuya Kida

Paper 560d: The Green Production Process of ε-Caprolactam with Vapor-Phase Beckmann Rearrangement

— **Hao Wang**, Shibiao Cheng, Yingqi Fan, Li Xie, Yusheng Jiang, Keyong Yang, Baoning Zong Paper 560e: Vapor-Phase Hydrotreating of Furfural over Ni-M/ SiO₂ Catalysts (M= Fe, Cu, Pt, Pd) for Propylene Production

- Sheng-Chiang Yang, Shawn D. Lin

Paper 560g: Hydrogenation of 2-Methylnaphthalene over Bi-Functional Supported Nickel Catalysts

— **Matthew J. Kline**, Sampath A. Karunarathne, Thomas J. Schwartz, M. Clayton Wheeler

Paper 560h: Kinetics Study of the Simultaneous Hydrodeoxygenation of Xylitol over a ReOx-Pd/CeO₂ Catalyst — Blake MacQueen, Jochen Lauterbach

Paper 560i: Novel Bio-Derived Solvents for Extraction of Natural Products — *Md. Anwar Hossain, Noppadon* Sathitsuksanoh

Paper 560j: Understanding and Improving the Recyclability of Supported Nickel and Cobalt Catalysts for the Deoxygenation of Bio-Derived Fatty Acids

— James M. Crawford, Courtney S. Smoljan, Jolie Lucero, Sarah F. Zaccarine, Nolan C. Kovach, Brian G. Trewyn, Svitlana Pylypenko, Moises A. Carreon

Paper 560k: Study on Catalytic Oligomerization of Glycerol over Alumina Supported Ca/La Mixed Oxides — Cheng-Yen Lin, Wei-Xiang Fang, Bing-Hung Chen

Paper 5601: Temperature Dependence of pH Dynamic Behavior in the Glucose Oxidase-Ferricyanide-Glucose-NaOH Reaction System in a CSTR

— **Lenka Schreiberova**, Barış Bager Solgun, František Muzika, Igor Schreiber

Paper 560m: Describing the Catalytic Role of Alkaline Earth Metals on Initiation during Cellulose Pyrolysis

— **Gregory G. Facas**, Vineet Maliekkal, Matthew Neurock, Paul Dauenhauer

Paper 560n: Towards Pharmaceutical Protein Stabilization: Insights from Theoretical Studies on Peptide Hydrolysis Reactions

— Katherine Lawson, Andrew J Adamczyk

Paper 560o: Computational Study on Biomass Fast Pyrolysis: Design Considerations for a Laboratory-Scale Fluidized Bed

— **Emilio Ramirez**, Tingwen Li, Charles E. A. Finney, Mehrdad Shahnam, C. Stuart Daw

Paper 560p: Ultrasound-Assisted Production of Ethyl Butyrate via a Lipase Cocktail

— Fernando C. de Sousa Filho, Roberto M. F. de Freitas, Bárbara K. N. Gadelha, Ellefson E. S. de Oliveira, Rodolpho R. C. Monteiro, Paula J. M. Lima, Maria C. M de Souza, José C. S dos Santos

Paper 560q: Food Waste Repurposing to an Integrated Biorefinery

- Elvis Ebikade, Dionisios G. Vlachos

Paper 560r: Mixed Al/B Catalysts: A Bifunctional Groups Modified Solid Acid Catalyst with Nano-Size Mesoporous for Efficient Conversion of Glucose to 5-Hydroxymethylfurfural in DMSO

— Jiangxiong Xiao, Jiayi Zheng, Shuxian Yuan, Zhitong Peng, Yao Liu, Xiaojie Zheng**, Xiaoqing Lin**

Paper 560s: Hydrothermal Catalytic Conversion of Biomass into Chemicals: Strategy and Mechanism — *Lingzhao Kong Sr.*

Paper 560t: Hydrothermal Carbonization of Microalgae for Hydrochar Production

— **Magdalini Tsarpali**, George Philippidis, John Kuhn

Paper 560u: Hydrogen Donation from Bio-Acids over Carbon Nano Tube (CNT) Based Bi-Functional Catalysts: Density Functional Theory Study

— **Jiajun Zhang**, Xiaolei Zhang

Paper 560v: Engineering Lignin Transformation Mechanisms to Create Value-Added Products Using Atomistic Modeling

— **Tanzina Azad**, Jonathan Schuler, Maria Auad, Thomas Elder, Andrew J Adamczyk

Paper 560w: Evaluation of AI, Ti, and Nb Oxides As Support for H₃PMo₁₂O₄₀ to be Used As Catalyst in Biodiesel Production from Low-Grade Oils

— L. Rafael V. Da Conceição, Ana Karine Carvalho, **Cristiano Reis**, Heitor Bento, Daniela Cortez, Heizir De Castro

Paper 560x: Effect of Process Parameters and Heterogeneous Catalysts on the Upgrading of Micro-Algal Bio-Crude Oil

— **Kodanda Phani Raj Dandamudi,** Tessa Murdock, Peter Lammers, Shuguang Deng

Paper 560y: Catalytic Transfer Hydrogenolysis of Xylitol over Bifunctional Pd-Based Catalysts — Qi Xia, Bin Yin, Xin Jin

Paper 560z: Catalytic Conversion of Glucose to Tartaric Acid over Au-Pt/TiO₂ Catalysts

— **Mengyuan Liu**, Tianqi Fang, Jie Ding, Xiaowen Ge, Hao Yan, Xin Jin, Chaohe Yang

Paper 560aa: Biofuel Production from Hydrotreatment of Fatty Acids Using Supported Ni/Mo Bimetallic Catalysts — Chao-Wei Lee, Po-Yi Lin, Bing-Hung

Paper 560ab: Large-Scale Exploitation of Glucose Reductive Aminolysis: Comparison of Jet-Loop and Trickle-Bed Reactor Performance

— **Jeroen Poissonnier**, Frederik Van Waes, Kristof Moonen, Guy B. Marin, Joris W. Thybaut

Paper 560ac: Characterization of Physical and Chemical Properties of Bio-Crude Oil from Hydrothermal Liquefaction of Food Waste — Hengameh Bayat, Mostafa

— Hengameh Bayat, Mostafa Dehghanizadeh, Feng Cheng, Catherine E. Brewer, **Umakanta Jena** Paper 560ad: Bifunctional Co-Mn Oxide Catalysts for Catalytic Transfer Hydrogenation of Levulinic Acid to γ-Valerolactone

— **Jinyao Wang**, Guangyu Zhang, Bin Yin, Hao Yan, Xin Jin

Paper 560af: Ionic Liquid-Mediated Rapid Catalytic Conversion of Lignocellulosic Grass to Biofuel Precursors in Microwave Reactors — Subhrajit Roy, Saikat Chakraborty

Paper 560ag: Main Effects Observed in the Conversion of Fructose in HMF
— Juliana Tacacima, Silas Derenzo,
Jogo G. R. Poco

Paper 560ah: Computer-Aided Analysis of Protease Catalytic Activity to Enhance Process and Product Development

— **Ashraf Ali**, Ashley Caroline Massey, Shounak Datta, Andrew J Adamczyk

Paper 560ai: Optimization of the Upgrading of Ethanol to n-Butanol Using in-Situ IR Spectroscopy in the Guerbet Reaction Network

— **Andreas Ohligschläger**, Nils van Staalduinen, Marcel A. Liauw

Paper 560aj: HMF Synthesis from Glucose By Reaction-Extraction System Using a Microreactor

— **Yosuke Muranaka**, Kenta Matsubara, Taisuke Maki, Shusaku Asano, Hiroyuki Nakaqawa, Kazuhiro Mae

Paper 560ak: Preparation of a New Enzymatic Biocatalyst Via the Taguchi Method: Application to Lipase a from Candida Artarctica Immobilized Onto Cashew Apple Bagasse

— Paula J. M. Lima, Juliana de F. Serpa, Bruna B. Pinheiro, Rodolpho R. C. Monteiro, Maria V.P. Rocha, Luciana R. B. Goncalves, José C. S dos Santos

Paper 560al: Reaction of Acetic Acid and Chicken Eggshells to Form Calcium Acetate

— **José A. Pérez**, Adriana M. Gómez, Cristian D. Hernández**, Luis Obregón**

Paper 560am: Enhanced Glucose Dehydration to 5-Hydroxymethyl Furfural through Encapsulated Phosphotungstic Acid in Metal Organic Frameworks

— Mohammad Shahinur Rahaman, Md. Anwar Hossain, Thanh Khoa Phung, Sarttrawut Tulaphol, Teerawit Prasomsri, Mark Crocker, Noppadon Sathitsuksanoh

Paper 560an: Coverage-Dependent First Principles Microkinetic Models for Copper-Catalyzed Hydrogenation of Carbonyl Groups: Role of Water and Sacrificial Alcohols

— **Jenoff De Vrieze**, Mark Saeys

Paper 560ao: Catalytic Deoxydehydration of Glycerol to Allyl Alcohol with 2-Hexanol As H-Donor – a Detailed Study of the Reaction Mechanism

— **Karen Silva Vargas**, Benjamin Katryniok, Marcia Araque Marin, Sebastien Paul, Franck Dumeignil Paper 560ap: Esterification of Isobutyl Alcohol and Acetic Acid - Kinetic Study — Felipe Martinez, Alvaro Orjuela, Gerardo Rodriguez

Paper 560aq: Sustainable Solutions for Selective Glycerol Oxidation into Dihydroxyacetone Using Commercial Catalysts

— **Pedro Walgode**, Rui Faria, Alírio E. Rodriques

Paper 560ar: Catalytic Conversion of Cellulose into Levoglucosenone Using Homogenous Brønsted Acid Catalysts in Polar Aprotic Solvents in a Flow Reactor — Alexa M. González-Rosario, Oscar Oyola-Rivera, Nelson Cardona-Martínez

Paper 560as: The Use of Aqueous Ethanol As a Solvent for the Catalytic Hydrogenation of Lactose to Lactitol — Andrew Kasick, Sunggyu Lee

Paper 560at: Influence of the Stirring System in the Scaled-up Transesterification to Produce Sucrose Esters Using a Solvent-Free Mixture — Maria F. Gutierrez, Andrea Suaza,

Alvaro Orjuela

Paper 560au: Aqueous Phase Reforming of Ethanol over Nickel Supported on Oxygen Ion Conducting Supports

— **Vincent Herrera**, Richard Nelson, Corey A. Leclerc

Paper 560av: Polyelectrolytes Enabled Co-Localization of Enzyme Cascades for One-Pot Synthesis

— **Zheyu Wang**, Junqian Wang, Gong Chen, Weina Xu, Zhongwang Fu, Guoqiang Jiang, Jianzhong Wu, Zheng Liu

Paper 560aw: Converting Biogas to Liquid Fuels By Low Energy Electrical Corona Discharge Processes

— **Yu Miao**, Alexandre Yokochi, Goran Jovanovic, Nick AuYeung, Annette von Jouanne, Ryan Collin, Ian Reddick, Andrew Traverso

Paper 560ax: Mechanisms of C-O and C-C Bond Activation of Acetic Acid Hydrodeoxygenation over Pt-Mo Catalysts

— **Yiteng Zheng**, Ziyu Tang, Simon G. Podkolzin

Paper 560ay: LaxBa₁-XFeO₃ Perovskite Oxide for Low Temperature Thermochemical Conversion of Carbon Dioxide

— **Hanzhong Shi**, Venkat R. Bhethanabotla, John N. Kuhn

Paper 560az: Hydroxyl-Mediated Ethanol Selectivity of CO₂ Hydrogenation — Chengsheng Yang, Rentao Mu, Jinlong Gong

Paper 560ba: H+ Conductivity and O₂ Impermeability of Ultrathin Oxide Layers with Built-in SiO₂ Separation Membrane for Scalable Artificial Photosynthesis

— Won Jun Jo

Paper 560bb: 3D Nitrogen-Doped Graphene Aerogel-Supported MnO Nanoparticles As Efficient Electrocatalyst for CO, Conversion to CO

— **Mengchu Wang**, Bike Zhang, Yao Shi, Yi He Paper 560bc: Non-Noble Metals Doped Bi-Nanoparticles for Electrochemical CO₂ Reduction

— Xue Han

Paper 560bd: Enhancing the Electrochemical Production of Syngas from Captured CO₂ by Using Silver Nano-Structured Electrocatalysts

— Omar Movil-Cabrera, Ningshengjie Gao, Tedd Lister, Luis Diaz-Aldana

Paper 560be: Electrochemical
Reduction of CO₂ on Transition Metal-P
Block Catalyst Compositions
— Sahithi Ananthaneni, Rees B.
Rankin

Paper 560bf: Synthesis and Characterization of Bimetallic Core@ Shell Structured Nanoparticles for Electrochemical Reduction of CO₂ into Formic Acid

— **Wei Jyun Wang**, Su Ha, Louis Scudiero

Paper 560bg: Copper-Nitrogen-Doped Carbon Nanostructures for an Efficient CO₂ Reduction Reaction

— **Huiyuan Cheng**, Xuemei Wu, Gaohong He

Siahrostami, Ian D. Gates

Paper 560bh: Doped Transition Metal Nitrides As Efficient Electrocatalysts for Electrochemical Reduction of CO₂ — Mohammadreza Karamad, Samira

Paper 560bi: Artificial Thylakoid to Coordinate Photo-Enzyme-Coupled Catalysis for Carbon Dioxide Upgrading — Shaohua Zhang, Jiafu Shi, Zhongyi Jiang

Paper 560bj: A Novel Approach to Kinetic Modeling of High Temperature CO₂ Adsorbents

— Michael A. Smith, Charles Coe, Anthony Vallace, Simon Brooks

Paper 560bk: Extrusion of Perovskite Oxide/ Silica Composites for Thermochemical Carbon Dioxide Conversion

— **Qian Li**, Hanzhong Shi, Venkat R. Bhethanabotla, John N. Kuhn

Paper 560bl: Understanding Mechanisms of CO₂ Electroreduction on Cu(100) with Kinetic Monte Carlo Simulations

— **Tianyou Mou**, Hemanth S. Pillai, Hongliang Xin

Paper 560bm: Promoting CO₂ Hydrogenation Activity and Methanol Selectivity of Cu/CeO₂ Catalyst By W-Doping

— Yong Yan**, Wen Liu**

Vlachos

Paper 560bn: A Computational Investigation of Catalytic Upgrading of CO₂ to Methanol over Indium Oxide — Maximilian R. Cohen, Dionisios G.

Paper 560bo: DFT Investigation of the Mechanism and Site Requirements for Reverse Water Gas Shift on Transition

Metal Sulfides

— Ronak Upadhyay, Lohit Sharma,
Jonas Baltrusaitis, Srinivas Rangarajan

Paper 560bp: Influence of Coordination Environment Around Anchored Single-Site Cobalt Catalyst for CO₂ Hydrogenation

— **Juan Jimenez**, Michael Royko, Jochen Lauterbach

Paper 560bq: Direct and Highly Selective Conversion of Carbon Dioxide into Chemicals

— Yuhan Sun

Paper 560br: Carbon Dioxide Hydrogenation

— **Sascha Kleiber**, Susanne Lux, Matthaeus Siebenhofer

Paper 560bs: Mesoporous Silica Supported Perovskite Oxide for Low Temperature Thermochemical CO₂ Conversion

— **Jeremy Brower**, Venkat R. Bhethanabotla, John Kuhn

Paper 560bu: Promoter and Support Effects on Transition Metal Carbides for CO₂ Hydrogenation

— **Mitchell B. Juneau**, Marc D. Porosoff

Paper 560bv: Carbon Dioxide
Activation and Synthesis of Cyclic
Carbonates, Followed By Aniline over
Hollowfibre Catalysts (HF-APS-Br)
— Abdo-Alslam Alwakwak, Ali
Rownaghi, Fateme Rezaei

Paper 560bw: Probing the Oxygen Evolution Reaction Efficacy of Pure and Doped NiOOH (0001) Using Hybrid Density Functional Theory

— **Ananth Govind Rajan**, John Mark P. Martirez, Emily A. Carter

Paper 560bx: Defect-Engineered Interface for Efficient Electrocatalyst — Kishwar Khan, Zhengtang Luo

Paper 560by: Mechanisms for Hydrogen Evolution on Transition Metal Phosphides and Pt

— **Chenyang Li**, Per Lindgren, Georg Kastlunger, Andrew A. Peterson, Tim Mueller

Paper 560bz: Multi-Task Machine Learning to Predict ORR Catalyst Descriptors and Performance across Surface Composition

— **Aini Palizhati**, Seoin Back, Kevin Tran, Zachary Ulissi

Paper 560cb: Post-Transition Metal Nanoparticles As Electrocatalysts for Nitrogen Reduction to Ammonia — Zihao Yan, Huiyuan Zhu

Paper 560cc: Isolated Diatomic Fe-Ni Metal-Nitrogen Sites for Synergistic Electroreduction of CO₂

— Yongheng Xiong, Qin Zhong

Paper **560cd**: Reutilization of Ba_{0.75}Sr_{0.25}CoNdO₆·O for Oxygen Reduction Reaction in Alkaline

— *Yi Zhang, Hongxia Qu*

Paper 560ce: Orbitalwise Coordination Number in Search of Metal Nanocatalysts for Oxygen Reduction — Siwen Wang, Noushin Omidvar, Emily Marx, Hongliang Xin Paper 560cf: Conversion of Glucose to Lactic Acid Using and Electrocatalytic Cell System

- Lars Ostervold III

Paper 560cg: The Role of Sulfur in CoSe(1-x)Sx for Enhanced Oxygen Electrocatalysis

— **Swetha Ramani**, Venkat R. Bhethanabotla, John Kuhn

Paper 560ch: Devisable Bottomup/ Top-Down Process Directed Facet-Engineered Pt Ni Porous Films As Efficient Oxygen Reduction Electrocatalysts

— Guanzhi Wang, Yang Yang

Paper 560ci: S-Doped Mop Nanoporous Layer for High-Efficiency Hydrogen Evolution Reaction

- Licheng Ju, Kun Liang, Yang Yang

Paper 560cj: Plasmonic Perovskite Semiconductor for Photoelectrochemical Water Splitting

— Zhao Li, Li Shi, Yang Yang

Paper 560cl: Exploratory Textual Data Analysis for Understanding the Research Development of Oxygen Reduction Reaction

— **Zheng Li**, Hongliang Xin

Paper 560cm: Electrochemical Oxidation of Methane at Platinum Electrodes Under Ambient Conditions

— **Michael Boyd**, Allegra A. Latimer, Colin Dickens, Adam Nielander, Christopher Hahn, Jens K. Norskov, Drew Higgins, Thomas F. Jaramillo

Paper 560cn: Transitional Metal
Coordinated with N-Doped Carbon
Nanofiber Integrated with Graphene for
the Oxygen Evolution Reaction in Acid
— Chaojun Lei, Lecheng Lei, Yang Hou

Paper 560co: Enhancing Organic Electrosynthesis through Artificial Intelligence: The Case of Adiponitrile Electrohydrodimerization

— Miguel Modestino, Daniela Blanco

Paper 560cp: The Role of Oxygen Incorporation in the Oxygen Reduction Reaction Activity of Molybdenum Nitride Catalysts

— Melissa Kreider, Michaela Burke Stevens, Yunzhi Liu, Alessandro Gallo, Anton levlev, Apurva Mehta, Robert Sinclair, Laurie A King, Thomas F. Jaramillo

Paper 560cq: Potential Dependent Kinetic Barriers of Oxygen Reduction Reactions (ORR) on Pt (111)

— **Shubham Sharma**, Andrew A. Peterson

Paper 560cr: Mechanistic Insights into Solution Phase Oxygen Reduction Reactions and the Effect of Metal Cation Dopants

— **Saurin H. Rawal**, William C. McKee, Benjamin Drewry, William A. Shelton Jr.. Ye Xu Paper 560cs: Effect of lonomer Coverage on Pt Electrocatalyst Performance in PEFCs

— **Timothy Van Cleve**, Mason Mooney, Guanxiong Wang, Sadia Kabir, K.C. Neyerlin

Paper 560ct: Atom-Thick Ir-Rich Skin on Ptir Nanocube Electrocatalysts for Efficient Ethanol Oxidation

— **Qiaowan Chang**, Shyam Kattel, Xing Li, Dong Su, Jingguang G. Chen, Zheng Chen

Paper 560cu: Ternary and Quaternary Microwave Synthesized Electrocatalyst for Ethanol Oxidation

- Shelby Foster, Lauren F. Greenlee

Paper 560cx: Multifunctional
Vanadium-Doped Cobalt Oxide Layer
on Silicon Photoanodes for Efficient
Photoelectrochemical Water Oxidation

Thun Xing Feng Ren Xiagfeng

— **Zhuo Xing**, Feng Ren, Xiaofeng Feng

Paper 560cy: A Microkinetic Analysis of the CO Electro-Oxidation Reaction on Pt Bimetallics: Understanding the Interplay of Bifunctional and Electronic Effects — Adam Baz, Adam Holewinski

Paper 560da: Analysis of PEFC

Cathode Catalyst Layer Based on Rate
Dependency on Oxygen Partial Pressure
— Miho Kageyama, Kazuhiro
Yamaguchi, Kento Takahashi, Yoshiyuki
Hashimasa, Tomoyuki Matsuda,
Motoaki Kawase

Paper 560db: Electrostatically Enhanced Catalytic Phase Transfer Hydrogenation of Acetophenone Under Low External Electric Field

— **Nan WANG**, Lawrence R. Weatherley

Paper 283b: Theoretical Study of Photocatalytic Water Splitting in a Tubein-Tube Setup

- Nopphon Weeranoppanant

Paper 560dc: Synthesis and Characterization of Pt-Zn Intermetallic Nanocatalysts for Light Alkanes Oxidative Dehydrogenation

— **Zhuoran Gan**, Muntaseer Bunian, William Sienicki, Sungsik Lee, Zheng Lu, Christopher L. Marshall, Yizhi Xiang, Yu Lei

Paper 560dd: Process Modified UV Assisted TiO₂ Adsorptive Desulfurization Mechanism Study

— Mingyang Chi, Bruce J. Tatarchuk

Paper 560de: Optimized Kinetic Parameters of Metallocene Catalyzed Olefin Polymerization through Modelling and Simulation

— Nikhil Prakash

Paper 560dg: Highly Stable and Coke Resistant Pt-Mn/K-Al₂O₃ Catalyst for Propane Dehydrogenation Reaction

— Madhav Sethia**, Nikita Dewangan**, Hidajat Kus, Sibudjing Kawi

Paper 560dh: A Novel Process for Selective O-Alkylation of Hydroquinone Using Methanol over Ionic Liquids — Priyanka Bhongale, Sunil Joshi, Nilesh Mali Paper 560di: Catalytic Ethylene Dimerization to 1-Butene Using Automated Construction of Microkinetic Models with RMG-Cat

— **Emily Mazeau**, Richard H. West, Katrin Blondal, C. Franklin Goldsmith

Paper 560dj: Metal-Promoted Dehydroaromatization of Ethylene over ZSM-5 Catalysts

— **Yunwen Zhou**, Hari Thirumalai, Lars C. Grabow, Jeffrey D. Rimer

Paper 560dk: Noble Bi-Metallic (Pt-Ru) Catalyst for Diesel Autothermal Reforming – Activity Tests and Characterizations

— **Jaemyung Lee**, Jiwoo Oh, Joongmyeon Bae

Paper 560dl: An Interesting Four-Stage Model of Au-Pd/TS-1 Bimetallic Catalysts for Direct Propylene Epoxidation with H₂ and O₂

- Zhishan Li, Weihua Ma, Qin Zhong

Paper 560dm: Model-Targeted Kinetic Experimentation for the Modeling of Industrial Ethylene Oxide Reactor

— **Şahin Sarrafi**, Stepan Spatenka, Mayank Patel, Yaşar S. Kabak, Sinan Üçyiğitler, Ahmet K. Avci, Fikret Inal

Paper 560dn: Kinetic Modeling of Catalytic Cracking of Paraffinic Naphtha with Molecular Mechanism

— **Ha-Nui Jo**, Kiwoong Kim, Jinsu Kim, Yoojin Han, Jae-Wook Shin, Young-Seek Yoon, In-Beum Lee

Paper 560do: Investigation of Ceria, Vanadia/Ceria and Gold/Ceria Catalysts By *Operando* Raman-Online FTIR during Toluene Oxidation

— Qingyue Wang, **Yingjian Luo**, King Lun Yeung, Miguel A. Bañares

Paper 560dq: Research on Bifunctional Catalysts for Hydrogen Production from Dimethyl Ether Steam Reforming

— Jinghong Lian, Changqing Guo, Hongyi Tan, Zhida Wang, Yan Shi, Zhuoxin Lu**, Changfeng Yan**

Paper 560dr: Assessing the Role of Zr-Al Interactions in Oxide-Grafted Zr Precursors for Ethylene Oligomerization Reactions

— **Galiya Magazova**, Joshua D. Wright, Neha Mehra, William F. Schneider, Jason C. Hicks

Paper 560ds: Mechanistic Understanding of the Role of Ga in the Dehydrogenation of Ethane on Ga/Al₂O₃ Catalyst

— **Sai Praneet Batchu**, Stavros Caratzoulas, Dionisios G. Vlachos

Paper 560dt: Effects of P and Metal Composition on the Performance of Mono- and Bimetallic Phosphides for Light Alkane Dehydrogenation

— Jessica A. Muhlenkamp, Jeonghyun Ko, William F. Schneider, Jason C. Hicks

Paper 560dv: Mechanism of Oxidative Dehydrogenation of Ethane at High Temperatures

— **Hilal Ezgi Toraman**, Gerhard R. Wittreich, Dionisios G. Vlachos

Paper 560dw: Self-Assembled Polymer Nanoreactors for Cascade Reactions — Andrew Harrison, Matthew Nguyen, Christina Tana

Paper 560dx: Towards Safe Process Intensification of Partial Oxidation Reactors: Theoretical Insights into Selective Ethylene Oxide Formation on Ag Catalysts

— **Siyuan Wu**, Bruce J. Tatarchuk, Andrew J Adamczyk

Paper 560dy: Microwave Catalytic Reactor for Converting Light Alkane to Aromatics

— **Xinwei Bai**, Brandon Robinson, Terence Musho, Casey Killmer, Yuxin Wang, Jianli Hu

Paper 560dz: Synthesis of High Purity Norbornene in a Microreactor Under Supercritical Conditions

— **Xin Xu**, Yin Wu, Bei Yuan, Zhen Yao, Kun Cao

Paper 560ea: Preparation, Characterization, and Performance Evaluation of High Performance Mesoporous Materials Based Hydrodesulfurization Catalysts

- Shakeel Ahmed

Paper 560eb: Isobutane Alkylation Kinetics with Mixed C₄ Olefins Catalyzed By Sulfuric Acid

— **Ling Zhao**, Weizhong Zheng, Piao Cao, Weizhen Sun

Paper 560ec: Influences of Metal-Modification and Lamellar Zeolite Structure on Ethylene to Liquid Aromatics Conversion Reaction Using MFI Catalysts

— **Luther Mahoney**, Laleh Emdadi, Dat Tran, Ivan Lee

Paper 560ed: Assessment of the Coke Deposited on Lamellar Metal-Modified MFI Zeolite Catalysts in the Transformation of Ethylene to Liquid Aromatics

— **Laleh Emdadi**, Luther Mahoney, Dat T. Tran. Ivan Lee

Paper 560ee: Synthesis,
Characterization and Mechanistic Study
of Structured Ga and Gapt Promoted
ZSM-5 in Ethane Dehydroaromatization
— Ashley Caiola, Brandon Robinson,
Xinwei Bai, Yuxin Wang, Jianli Hu

Paper 560ef: Machine Learning Discovery of Mo₈V₂Nb₁-Based Mixed-Oxide Catalysts for Controlled Partial Oxidation of Ethane

— **Musa O. Najimu**, Juan Jimenez, Michael Royko, Travis Williams, Jochen Lauterbach, Erdem Sasmaz

Paper 560eg: Core-Shell Structured Mixed Metal Oxides for Oxidative Dehydrogenation of Ethylbenzene Under a Cyclic Redox Scheme

— Xing Zhu, **Yunfei Gao**, Xijun Wang, Vasudev Pralhad Haribal, Junchen Liu, Fanxina Li

Paper 560eh: Selective Hydrogenation of Acetylene to Ethylene over Bi-Metallic Catalysts

— **Qingyuan Li**, Yuxin Wang, George Skoptsov, Jianli Hu Paper 560ei: Catalyst Development for Oxidative Coupling of Methane in a Gas-Solid Vortex Reactor

— **Saashwath Swaminathan Tharakaraman**, Guy B. Marin, Mark Saevs

Paper 560ej: Impact of Ni and Mg Loadings on Dry Reforming Performance of Pt/Ceria-Zirconia Catalysts

— **Yetunde O. Sokefun**, Babu Joseph, John N. Kuhn

Paper 560ek: Kinetics of O₂ Activation over Cu-Exchanged Zeolites: Implications for Partial Methane Oxidation

— **Daniel T. Bregante**, Laura N. Wilcox, Rajamani Gounder, David Flaherty

Paper 560el: Effect of Promoter Loading on Iron Supported Fischer-Tropsch Synthesis Catalyst at High-Temperature

— **Yajing Chang**, Sreya Seby, David Weber, Babu Joseph, John N. Kuhn

Paper 560em: Mechanistic Origins of the High-Pressure Inhibition of Methanol Dehydration Rates in Small-Pore Acidic Zeolites

— John R. Di Iorio, Alexander Hoffman, Claire T. Nimlos, Steven V. Nystrom Jr., David Hibbitts, Rajamani Gounder

Paper 560en: Fischer-Tropsch Synthesis on Natural Zeolite-Supported Fe Catalysts

— **Joshua Gorimbo**, Roick Chikati, Adolph A. Muleja, Diakanua Nkazi

Paper 560eo: A One-Step Method of Durene Synthesis Directly from Syngas Using Integrated Catalyst of Cu/ZnO/ Al₂O₂ and Co-Nb/HZSM-5

— Minzhe Li

Paper 560ep: Metal-Containing ZSM-5
Catalysts for the Dry Reforming of
Methane: Exploring Synergistic Effects

Meson Hoffman Carlos Carroro

— **Megan Hoffman**, Carlos Carrero, Raj Thakur, Justin Smith

Paper 560er: Long-Term Stability of Modified Ferrite Catalysts for High-Temperature Water-Gas Shift Reaction at Elevated Pressures

— Devaiah Damma

Paper 560es: Size Effect of $\mathrm{Co_3O_4}$ -Supported Pd Nanoparticle on the Catalytic Activities of CO Oxidation and Water-Gas Shift

— **Rui Huang**, Kyeounghak Kim, Myeong Gon Jang, Jeong Woo Han

Paper 560et: Hydrogenation of Dimethyl Oxalate to Ethylene Glycol over Mesoporous Silica Supported Copper Catalysts

— Xinbin Yu, Christopher Williams

Paper 560eu: High Yield to Lower Hydrocarbon in FT Synthesis: Based on Melting Effects on Znfe Spinel

— **Wenlong Song**, Huiqiu Wang, Yilin Hou, Zhaohui Chen, Dali Cai, Weizhong Qian Paper 560ev: Fischer-Tropsch Synthesis in Microscale-Based Reactor, Experimental and Mathematical Modeling

 Yousef Alanazi, Omar Mohamed, Andrew Traverso, Alexandre Yokochi, Goran Jovanovic

Paper 560ex: Kinetic Monte Carlo Study on Multi-Facet Copper Catalytic Surface for Efficient Methanol Synthesis

- Jiyeong Cho

Paper 560ey: Methane Pyrolysis in Molten Metal/Salt Two-Phase Reactors

— **Nazanin Rahimi**, Dohyung Kang, John Gelinas, Aditya Menon, Michael Gordon, Horia Metiu, Eric McFarland

Paper 560ez: Carbonylation of Dimethyl Ether over H-Mor: Elucidating the Effects of Acid Strength

— Kai Cai, Xinbin Ma, Shouying Huang

Paper 560fa: DFT Modeling of Liquid Solvent Effects on the Catalytic Surface Reactions in Fischer-Tropsch Synthesis

— Alireza Asiaee, Kenneth M. Benjamin

Paper 560fb: An Effective Microkinetic Modelling Strategy for Direct DME Synthesis from Syngas over Hybrid Cza/ FER Catalyst

— **Jongmin Park**, Myung-June Park, Won Bo Lee, Jong Wook Bae

Paper 560fc: Multi-Stage Fluidized Bed Technology for Methanol to Aromatic — Yilin Hou, Zhaohui Chen, Wenlong Song, Weizhong Qian

Paper 560fd: Combined DFT and Microkinetic Study of Dry Reforming of Methane on Ni and B Promoted Ni Surfaces

— **Ojus Mohan**, Shambhawi Shambhawi, Alexei Lapkin, Samir H. Mushrif

Paper 174ci: Determination of Kinetics for Methane Dry Reforming Using Plasma

— **Cassiane O. Martins**, Frédéric Marias, Jean-Paul Robert-Arnouil, Stephanie Moyal

Paper 560fe: Catalytic Incineration of Volatile Organic Compounds on Pd/ MnO₂-CeO₂ Catalysts

— Yu-Wen Chen

Paper 560ff: Core-Shell Pt/Al₂O₃@ Cu/ZSM-5 Catalyst for Ammonia Slip Catalyst in Diesel Aftertreatment

— **Ghosh Rajat**, Michael Harold, Thuy T. Le, Jeffrey D. Rimer, Di Wang

Paper 560fg: The Role of Noble Metals (M=Rh,Pd,Ag,Au,Pt) Promoting Active Oxygen Enhancing Soot Oxidation in CeO₂ Vacancy: Experiment with Tight Contact and a DFT Study

— **Deok Yeon Jo**, Jae Hwan Lee, Kwan-Young Lee

Paper 560fh: An Experimental Verification of Pressure Drop for Removal of VOC

— **David Jecha**, Vladimir Brummer

Paper 560fi: Impact of Copper Exchange Protocol on Cu-CHA SCR Activity

— **Aibolat Koishybay**, Chun-Te Kuo, Kyle Groden, Ayman M. Karim, Jean-Sabin McEwen, Daniel F. Shantz

Paper 560fj: First-Principles Studies of CO Oxidation on MgAl₂O₄ Supported Iridium Single Atoms

— **Jiamin Wang**, Yubing Lu, Ayman M. Karim, Hongliang Xin

Paper 560fk: Photocatalytic Degradation of NOx Using CNT-TiO₂ Nanocomposites

— **Bailey McAuley**, Brian Everhart, Ahmed Abdulrazzaq Qasim Al Mayyahi, Placidus B. Amama

Paper 560fl: A Temporal Analysis of Products (TAP) Study of Passive NOx Adsorption (PNA) on 1% Pd/SSZ-13

— **Unmesh Menon**, Hari Thirumalai, Bhuiyan Md. Rahman, Abhay Gupta, Michael Harold, Lars C. Grabow

Paper 560fm: The Effect of Polyethylene Glycol Modification on CrOx/TiO₂ Catalysts for NO Oxidation — Fanyu Meng, Shule Zhang, Qin Zhong

Paper 560fn: Catalytic Oxidation of Volatile Organic Components (VOCs) over Silver Nanoparticles Dispersed in Monodisperse Titania Nanospheres

— Adarsh Bhat, Alexander Hill, Pallav Jani, Hiroko Ohtani, Kevin Ellwood, Johannes W. Schwank

Paper 560fo: Mechanistic Study of Water Oxidation to Ozone on Rutile SnO₂ (110) with Computational Chemistry — Charles Griego, Angela Leo, Karthikeyan Saravanan, John A. Keith

Paper 560fq: Enhanced CO and C_3H_6 Conversions on Spinel Catalysts: Impact of Catalyst Architecture

— **Zhiyu Zhou**, Michael Harold, Dan Luss

Paper 560fr: One-Pot Synthesis of Gold Embedded Ceria Nanoshapes for Catalytic NO Reduction By CO — Meijun Li, Xuanyu Zhang, Sheng

Paper 560fs: Advancement of Nerve-Agent Filters, Polyoxometalates, By Utilizing a Correlated Multimodal

Dai 7ili Wu

Approach
— Yiyao Tian, Anna M. Plonka, Amani
Ebrahim, Daniel L. Collins-Wildman,
Craig L. Hill, Anatoly I. Frenkel

Paper 560ft: Designing of a New Prototype to Detoxify Carcinogenic Cr(VI) Metal from Drinking Water — Tuhin Kumar Maji, Samir Kumar Pal

Paper 560fu: Chemical Warfare Agent Simulant Degradation over Metal Nanoparticles Supported on TiO₂ Aerogels

— **Ashley M. Pennington**, Paul A. DeSario, Catherine L. Pitman, Debra R. Rolison, Jeremy J. Pietron

Paper 560fv: Fabrication of Natural Clay Based Nanocomposite Materials for Advanced Catalytic Treatment of Organic Pollutants in Wastewater — Adolph A. Muleja, Mukuna P. Mubiayi, Bhekie B. Mamba

Paper 560fw: Photocatalytic Metal Organic Framework Induced Ag Nanoparticles Composites for Phenol Detection

- Qian Liu, Cerasela Zoica Dinu

Paper 560fx: Enhancement of Heterogeneous Silver and Copper Catalysts Stability for Catalytic Ozonation in Water

— Wenwen Yang, Zheng Lu, Zhuoran Gan, Muntaseer Bunian, Xiankun Chen, Bernhard Vogler, Steve Heald, Tingting Wu, Yu Lei

Paper 560fy: Impact of Defects on the Decomposition of Chemical Warfare Agent Simulants in Zr-Based Metal Organic Frameworks

— **Minh Nguyen Vo**, Jonathan Ruffley, J. Karl Johnson

Paper 560fz: Fabrication and Performance Evaluation of Photocatalytic Reactor for the Removal of Malathion from Waste Water

— Sachin Mohan, Mohammed Ijas

Paper 560ga: Insights into H₂S Catalytic Oxidation Performance on Activated Carbon Supported Cu-Based Catalyst at Room Temperature

— **Feiyue Fan**, Long Zhao, Hong Hou

Paper 560gb: The Synergistic Effect of Copper and Niobium Species on a Novel Ti-Based Ternary Oxide Catalyst for NO_x Removal with NH₂

— **Xiaoxiang Wang**, Su-Jing Li, Wei Li, Yao Shi

Paper 560gc: Surface Lattice Oxygen Activation Via Zr₄ * Cations Substituting on a₂ * Sites of MnCr₂O₄ Forming ZrxMn₁ * xCr₂O₄ Catalysts for Enhanced NH₃-SCR Performance

— Erhao Gao, Yi He

Paper 560gd: Degradation of Gas-Phase O-Xylene Via Non-Thermal Plasma over Fe Doped LaMnO₃ Catalysts: the Byproducts Control — *Tianyu Shou*, *Yao Shi*, *Yi He*

Paper 560ge: Recent Progresses in Enhancing the Hydrothermal Stability of Cu-SSZ-13 Catalyst for Selective Catalytic Reduction of NOx with NH₃ — Yongdan Li

— Tongaan Li

Paper 560gf: Catalytic Oxidation of VOC – Modelling, Reactor Design and Industrial Off Gas Treatment

— Vladimir Brummer, David Jecha

Paper 560gg: Improved Catalytic Performance of (RE, TM) Co-Doped Ceria for CO Oxidation

— **Hyung Jun Kim**, Dongjae Shin, Jeong Woo Han

Paper 560gh: Metal Oxide Catalysts for Low Temperature NOx Adsorption — Raghav Kaushik Siddavaram, Huawang Zhao, Xiaoyin Chen, Johannes W. Schwank Paper 560gi: Surface Redox-Acid Pair Sites Required for Achieving High Performance for the Selective Catalytic Reduction of NOx with NH₃

— Li Cao, Shaohua Xie, **Ge Song**, Xiaodong Wu, Fudong Liu

Paper 560gj: A Waste-to-Value Technology for Sustainable Bromine Production Using Heteroatom-Doped Carbon Nanostructures

— **Deeksha Jain**, Jonathan Hightower, Dishari Basu, Vance Gustin, Anne Co, Aravind Asthagiri, Umit S. Ozkan

Paper 560gk: Descriptor-Based Modeling of CO Oxidation over Alumina-Supported Single Metal Atoms

— Konstantinos Alexopoulos, Dionisios G. Vlachos

Paper 560gl: Selective Oxidations of Alkanes Via Gas-Phase Catalytic Cycles of NOx in Alkane-O₂-NO Mixtures
— Annamalai Leelavathi, Yilang Liu,

Prashant Deshlahra

Paper 560gm: Flame-Synthesized Pd-TiO₂ Catalyst for Oxygen Removal from Oxy-Coal Combustion Flue Gas

— **Sungyoon Jung**, Nathan Reed, Gregory Yablonsky, Pratim Biswas

Paper 560gn: Modeling and Experiments of Coal Combustion and its Blends with Woody Biomass in a 1.5 MW Roiler

— **Seyedhassan Fakourian**, Jinze Dai, Kevin Whitty, Andrew Fry

Paper 560go: Regeneration of Ptsoxtizr/SiO₂ By Hydrogen Treatment. Part II Catalyst Regeneration in a Semibatch Fluidized Bed Reactor

— Roberto E. Galiasso Tailleur, Carlos Farina

Paper 560gp: In-Situ X-Ray Absorption Spectroscopy (XAS) Study on Bimetallic Iron-Nickel Based Nanoparticles for Oxygen Evolution Reaction (OER) Catalysis

— **Prashant Acharya**, Ryan H. Manso, Laszlo Kekedy Nagy, Sergio I. Perez Bakovic, Jingyi Chen, Lauren F. Greenlee

Paper 560gq: Structure-Property Relations of PtWOx/C Inverse Catalysts — Jiayi Fu, Weiqing Zheng, Shizhong Liu, Cong Wang, Stavros Caratzoulas, Raymond J. Gorte, Dionisios G. Vlachos

Paper 560gr: Annealing Studies of Cobalt Supported on Hydrothermally Synthesised Carbon Spheres for Fischer-Tropsch Synthesis

— Mahluli Moyo

Paper 560gs: Design and Evaluation of Nanostructured Doped Perovskite Oxygen Carriers

— Christopher L. Hanselman, Dominic Alfonso, Jonathan W. Lekse, De Nyago Tafen, Christopher Matranga, David C. Miller, Chrysanthos E. Gounaris

Paper 560gt: Synthesis of Zeolite-Encapsulated Metal Nanoparticles Via a Cationic Polymer-Assisted Strategy for Substrate-Selective Catalysis

- Hong Je Cho, Bingjun Xu

Paper 560gu: High Performance Enzymatic-Transesterification in an Anhydrous Gas Flux Using Lipase Encapsulated in Graphene Oxide Aerogel

— Weina Xu, Zhongwang Fu, Gong Chen, Zheyu Wang, Yupei Jian, Yifei Zhang, Diannan Lu, Guoqiang Jiang, Jianzhong Wu, Zheng Liu

Paper 560gv: Rational Catalyst Design: Kinetics Put into Action for Small Open Data

— **Pedro S.F. Mendes**, Sébastien Siradze, Laura Pirro, Joris W. Thybaut

Paper 560gw: Novel Nanostructured Transition Metal Oxides for Catalysis — *Yulian He*

Paper 560gx: Defect Engineering of in-Situ Exsolved Nanoparticle Catalysts on Perovskite Supports

— **Soham Shah**, Samuel Sayono, Kandis L Gilliard Abdul-Aziz

Paper 560gy: Characterization of Cyclodextrin-Based Metal-Organic Frameworks with Catalyst Molecules — Anna Nagai, Wataru Michida, Mina Sakuraqi, Katsuki Kusakabe

Paper 560gz: Surface Phase Diagrams of Strontium Titanium Oxide Using an Automated Ab-Initio Grand Canonical Monte Carlo Method

— **Vignesh Bhethanabotla**, Robert Wexler, Andrew M. Rappe

Paper 560ha: Regeneration of PtSO ZrTi/SiO₂ By Hydrogen Treatment. Part I. Spent Catalyst Characterization — Roberto E. Galiasso Tailleur, Carlos Farina, Rough P. Ronaldi

Paper 560hb: Hydrogen and Carbon Nanomaterials Production from Pyrolysis of Waste Plastics with Bimetallic Catalyst: Product Characterization and Formation Mechanism

- Dingding Yao, Chi-Hwa Wang

Paper 560hc: In Situ Synthesis of Zn-Doped Ordered Mesoporous Carbon: Structure Characterization and Catalytic Performance Evaluation

— Baohe Wang, Huanhuan Han, Jing Zhu**, Jing Ma**

Paper 560hd: Development of an Accelerated Deactivation Protocol for Vacuum Gasoil Hydrocracking Catalysts — July Carolina Vivas Báez, Gerhard D. Pingruber, Alberto Silva Servia, Anne-Claire Dubreuil, David de Jesús Perez Martinez

Paper 560he: Investigation on Control of Surface Reactivity Towards Carbon, Oxygen, and Hydrogen of Intermetallic Compounds in Wet Reforming of Hydrocarbons and Oxygenates

— **Yuanjun Song**, Yang He, Siris Laursen

Paper 560hf: Dual Role of Surfactants in Zeolite Synthesis and Catalyst Optimization

— **Aseem Chawla**, Noemi Linares, Rui Li, Rishabh Jain, R. John Clark, James Sutjianto, Jeremy C. Palmer, Javier García-Martínez, Jeffrey D. Rimer **Paper 560hg:** Elucidating the Factors Governing the Organic-Free Interzeolite Transformation

- Rishabh Jain, Jeffrey D. Rimer

Paper 560hh: In Situ Analysis and Dynamic Response Surface Modeling of Energetic Material Hydrolysis

— **Eric Gauthier**, Edward Cooke, Peggy Sanchez, Melissa Jablonski

Paper 560hi: Understanding Molecular Structural Changes in Sulfated Mixed Metal Oxides

— Justin Marlowe, Adam Zuber, Aditya Khandare, **George Tsilomelekis**

Paper 560hj: Fin-like Zeolite Catalysts: A New Class of Hierarchical Materials — Heng Dai, Yufeng Shen, Donglong Fu, Thuy T. Le, Taimin Yang, Matthias Filez, Xiaodong Zou, Bert M. Weckhuysen, Jeffrey D. Rimer

Paper 560hk: Exploration of Si-Based Precursor Pyrolysis with Theoretical and Experimental Studies of Semiconducting Nanomaterial Properties

— **Yeseul Choi**, Anjitha S. Geetha, Christian Martin, Guro M. Wyller, Thomas J. Preston, Andrew J Adamczyk

Paper 560hl: Raman-Spectrokinetics to Gain Insights on Support Effects of Supported Vanadium Oxide Catalysts — Jorge Moncada, Kaitlyn Lawrence, William R. Adams, Carlos A. Carrero

Paper 560hm: Nitrogen-Doped Carbon: A Support to Synthesize Ultra-Small and Stable Pt-Nanoparticles

— **Fahim Rahman**, Huynh Ngoc Tien, Hector Colon-Mercado, John R. Regalbuto

Paper 560hn: Reactions of Methyl and Ethyl Fragments on α-Cr₂O₃(101⁻2)

— Han Chen

Paper 560ho: Colloidal Gold Nanoparticles for Catalytic Applications — *Chinmay Joshi, Saptarshi Chakraborty*

Paper 560hp: Coupling the Magnetic and Catalytic Properties of Fe₃O₄ Via Shape-Controlled Routes and Cr Doping — Natalia da Silva Moura, Bradley Watson, Hunter Simonson, Pragathi Darapaneni, Kerry M. Dooley, James A. Dorman

Paper 560hq: Synthesis of Supported Metal Nanoparticles By Controlling the Interaction between Colloidal Metal Nanoparticles and Supports

— **Laibao Zhang**, David Cullen, Kunlun Ding

Paper 560hr: Development of Secondary Phase in Various Zeolites Framework

— Safa Gaber, Dina Gaber, **Georgia Basina**, Alya Alzaabi, Alyaa Alzaabi, Meera S. Alqemzi, Fatima Abdullah, Aziza Alameeri, **Yasser Al Wahedi**

Paper 560hs: Synthesis of Well-Defined Heterogeneous Catalysts Using Atomic Layer Deposition

— **Bochuan Song**, Helena Hagelin-Weaver Paper 560hv: Initial Stages of Chloride Enhanced Depassivation of Chromium Protected Layer, a Density Functional Theory Study

— **Kofi Oware Sarfo**, Pratik V. Murkute, Yongfeng Zhang, O. Burkan Isgor, Julie D. Tucker, Liney Arnadottir

Paper 560hw: Engineering Dopant Position in Core-Shell CeO₂-ZrO₂ Nanoparticles to Control Catalytic Activity

— **Behnam Safavinia**, Pragathi Darapaneni, Orhan Kizilkaya, David Cullen, Jarod Larriviere, Kerry M. Dooley, James A. Dorman

Paper 560hx: Role of Support Reducibility in the Catalytic Activity of CO Oxidizing Reactions on Pd Loaded Cu-Doped Ceria

— **Dongjae Shin**, Myeong Gon Jang, Jeong Woo Han

Paper 560hy: Contact Angle Measurements of Binary Mixtures for Determination of Surface Free Energy — Ziyang Zhang, Ping He, Michael T. Timko, Christopher Lambert

Paper 560hz: Sequential $\rm H_2$ -CO Pulse Chemisorption for Estimating in-Situ Ni Dispersion : Application on ALD-Coated Catalyst

— **Shaik Afzal**, Anuj Prakash, Patrick Littlewood, Tobin J. Marks, Eric Weitz, Peter C. Stair, Nimir Elbashir

Paper 560ia: Kinetic Modelling of the Ammonia Temperature Programmed Desorption of ZSM-5

— Rebecca Gibson, **Mark Simmons**, Athanasios Tsolakis, Hugh Stitt, Stephen Schuyten, Robert Gallen

Paper 560ib: To Leach or Not to Leach? Combined Data Analysis to Elucidate the Leaching Behavior of Strongly Acid Resin Supported Pd and Pdco NP Catalyst in Suzuki Coupling

— **Beau Van Vaerenbergh**, Jeroen Lauwaert, Joris W. Thybaut, Pieter Vermeir, Jeriffa De Clerca

Paper 560id: An Ambient Pressure XPS Study of Methane Dissociation and Oxidation on IrO₂(110)

— **Rachel Martin**, Vikram Mehar, Christopher Lee, Stefano Albertin, Uta Hejral, Lindsay Merte, Edvin Lundgren, Jason F. Weaver

Paper 560ie: Demonstrating the Power of Custom Modeling Integrated into Flowsheet Simulation

— **Reza Haghpanah**, Evan Bergman, Brad Metzler

Paper 560if: Generalized Adsorption Models on Metal Nanoparticles — James Dean, Michael G. Taylor, Giannis Mpourmpakis

Paper 560ig: Enhancing Ab Initio Microkinetic Models with Machine Learning

— **Huijie Tian**, Srinivas Rangarajan

Paper 560ih: Catalyst Design for Glycerol Valorization through Data Science, First Principles Modeling, and Experimental Verification

- Shenggang Li

Paper 560ii: Coupling Experimental Kinetics and Thermodynamic Modeling with IR Spectroscopy and Machine Learning for Fundamental Studies and Fast Product Quantification

 Natalia Rodriguez Quiroz, Joshua Lansford, George Tsilomelekis, Dionisios G. Vlachos

Paper 560ij: Elucidating Reaction Pathways through Combined Insights from Experimental and Computational Hammett Analysis

— Shaama Mallikarjun Sharada

Paper 560ik: Reaction Mechanism Modeling of By-Products in Semiconductor Manufacturing Process Using Reaction Mechanism Generator (RMG)

Dongju Kang

Paper 560il: Molecular Dynamics Simulation of Graphene Oxide-Enzyme Assembly for Gaseous Catalysis

— **Zhongwang Fu**, Gong Chen, Weina Xu, Lu Diannan, Jianzhong Wu, Zheng Liu, Zheyu Wang

Paper 560im: The Development and Application of Novel Yolk@Shell Materials to CO₂ Recycling

— Cameron Álexander Hurd Price, Laura Pastor-Perez, Tomás Ramirez-Reina, Jian Liu

Paper 174as: Theoretical Investigations of Lewis Acid-Catalyzed Alkane C-H Activation in Metal-Modified Zeolites

— **Erum Mansoor**, Martin Head-Gordon, Alexis Bell

Paper 560in: An Investigation into the Catalytic Cycle of Cytochrome P-450 Involving 1-n-Alkyl-3-Methylimidazolium Cations As Substrate

— Atiya Banerjee, Jindal K. Shah

Paper 560jg: Effect of Pd Precursors on Pd/TiO₂ Catalysts Prepared by Different Methods and Their Catalytic Activity in Hydrogenation of Maleic Acid

— **Ye Eun Kim**, Mi Yeon Byun, Jae Ho Baek, Kwan-Young Lee, Man Sig Lee

Paper 560io: Design, Synthesis and Evaluation of Ir@Pt Bimetallic Catalysts for High Temperature Decomposition of SO₃ to SO₂ in the HyS Process for Thermochemical Water Splitting

— **Weijian Diao**, John Meynard M. Tengco, Fahim Rahman, John R. Monnier, John R. Regalbuto, Daniel M. Ginosar, Birendra Adhikari, Claudio Corgnale

Paper 560ip: Metal-Organic Framework Templated Catalysts for Hydrogen Generation from Low-Temperature Ammonia Decomposition

— Zhigang Hu

Paper 560iq: Solid-Solid Reactions: A Variation on a Classical Theme

— **Minakshee Phutke**, Akkihebbal K. Suresh

Paper 560ir: Modeling of Transport-Kinetic Interactions in Various Design Configurations of Egg-Shell Catalyst Particles

— Anuradha Nagaraj, Patrick L. Mills

Paper 560is: Mechanism of Effluence of Internal Substance from Pluronic Micelles By External Stimuli

— **Daisuke Kobayashi**, Daiki Takemi, Atsushi Shono

Paper 560it: DESI-MS Based High Throughput Reaction Screening to Guide Bulk/Microfluidic Chemistry: A Correlation Analysis between Droplet and Bulk/Microfluidic Reaction Systems

— **Botond Szilagyi**, Zinia Jaman, David Logsdon, Harrison S. Ewan, Christina E. Ferreira, Tiago JP Sobreira, David H. Thompson, Robert G. Cooks, Zoltan K. Nagy

Paper 560iu: Understanding the Promotional Effects of Acids and Halides on Direct Synthesis of H₂O₂ and Their Effect on the Nature of Catalytically Active Pd — Pranjali Priyadarshini, David

Paper 560iv: Studying Heterogeneous Cobalt Catalysts for Sulfite Oxidation to Compare with Theoretical Models — Zachary Watson, Joseph Veglak, Gregory T. Neumann

Paper 560iw: Distinguishing Homogeneous and Heterogeneous Catalytic Pathway in Cuprous Oxide Nanoparticle-Catalyzed C-C Coupling

— **Ravi Teja Addanki Tirumala**, Marimuthu Andiappan

Reactions

Paper 560ix: Synthesis of Tetrapropylammonium Bromide (TPABr) — *Utkarsh Maheshwari*, *Vinit Ponkshe*, *Ashwin Ponnapan*

Paper 560iy: Periodic Operations of a CSTR with Flow-Rate Modulations — Using the Nonlinear Frequency Response Method for Finding the Best

Strategy
— *Menka Petkovska*

Paper 560iz: Bifurcation Analysis of Coupled Homogeneous-Heterogeneous Reactions in Monolith Reactors

— **Bhaskar Sarkar**, Vemuri Balakotaiah

Paper 560ja: Validated CFD Simulations of a Bench-Scale Fixed Bed Fischer-Tropsch Reactor

— **Jianqi Shen**, Wei Hua Ho, Xinying Liu, Diane Hildebrandt

Paper 560jb: Two-Dimensional Heterogeneous Reactor Model for an Exothermic Reaction Exhibiting Deactivation By Fouling: Modeling and Computational Strategy

— Javier Ibáñez Abad, **Jeroen Poissonnier**, Joris W. Thybaut

Paper 560jc: Modeling of Polymerization of Methyl Methacrylate in Homogeneous Systems As a Framework for Processes Improvements

— **Antonio C. O. Intini**, Reinaldo Giudici

Paper 560jd: Tributyl Citrate Production from Calcium Citrate: Solid-Liquid Reaction Kinetics

- Andres F. Cabeza, Alvaro Orjuela

Paper 560je: Mechanism and Kinetics of Metal Dissolution in Nitric Acid

— G. Vamsi Vikram, S. Pushpayanam

Paper 560jf: Dynamic Catalysis As

an Emerging Strategy in Reaction Engineering

— **M. Alexander Ardagh**, Omar A. Abdelrahman, Qi Zhang, Paul Dauenhauer

(561) Poster Session: Concentrated Solar Energy for Power Generation and Chemical Processing

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Alexandre Yokochi, Chair Nick AuYeung, Co-Chair Wojciech Lipinski, Co-Chair Christopher L. Muhich, Co-Chair

Sponsored by: Concentrated Solar Energy for Power Generation and Chemical Processing

Paper 561a: Modal Switching for Continuous Solar Reforming — Lucas Freiberg, Fuqiong Lei, Nick AuYeung

Paper 561b: Experimental Study on a Solar Falling-Film Photochemical Hybrid System for the Decolorization of Azo Dyes

— **Miao Chen**, Hongxun Hao

(562) Poster Session: Environmental Division

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Jeffrey R. Seay, Chair Sage R. Hiibel, Co-Chair Debalina Sengupta, Co-Chair

Sponsored by: Environmental Division

Paper 562a: Effects of Cadmium and Mercury on the Germination of Lolium Perenne

— Yuby Cruz, Jorge L. Gallego, Carolina Montoya-Ruiz, **Juan F. Saldarriaga Sr.**

Paper 562b: Analysis of the leachates of the monoliths from cementhazardous waste ash mixture

— Ana M. Barbosa, Julieth E. Romero, Yuby Cruz, Juan D. Alonso, Ximena Gaviria, **Juan F. Saldarriaga Sr.**

Paper 562c: An Integrated CO₂ Capture and Conversion Device based on Metal-Organic Framework -and Cu Nanostructured Electrocatalyst — Nedal N. Marei, Md G. Kibria, George K. Shimizu

Paper 562d: Triboelectric Particulate Matter Purifier Using Electrospun Ethyl Cellulose

— Minhee Cho, Jeong Gil Seo

Paper 562e: The Application of a Box-Behnken Design in the Study of Microcystin Production

— **Gisella Lamas-Samanamud**, Fabiano Naves, Carla Loures, Tony Reeves, Heather Shipley Paper 562f: Surface Change of Lean-NOx Trap Adsorbent through CuO Co-Impregnation and Its NOx Storage-Desorption Performance

— **Hyunwook Kim**, Ki Bong Lee

Paper 562g: Measurement of Hansen Solubility Parameter on Pollen Particle Surface and Application to Pollen Removal in Air

— **Yuki Kato**, Shinichi Tsutsumi, Nobuyuki Fujiwara, Hideki Yamamoto Sr.

Paper 562h: Design of a Hierarchical Fe-ZSM-5@CeO₂ Catalyst and the Enhanced Performances for the Selective Catalytic Reduction of NO with NH₂

- Liang Chen

Paper 562i: Evaluation on the Removal Performance of Dichloromethane and Toluene from Waste Gases Using an Airlift Packing Reactor

— Peilun Xu

Paper 562j: Preparation of Flexible Denim-Derived Activated Carbon Cloths for Environmental and Electrochemical Applications

— **Tomás Cordero-Lanzac**, Francisco J. García-Mateos, Juana M. Rosas, José Rodríquez-Mirasol, Tomás Cordero

Paper 562k: Hexavalent Chromium Removal from Treated Water Via Electrospun Composite Nanofibers

— Yang Lu, Jesse Horne, Joshua Perch, Zhanhu Guo, **Evan K. Wujcik**

Paper 562m: CO₂ Utilization By Calcium Carbonate, Magnesium Carbonate and Sodium Bicarbonate Production Using Metal Cations in Reject Brine Solutions

— **Dongwoo Kang**, Yunsung Yoo, Injun Kim, Jinwon Park

Paper 562n: Inverse Vulcanized Polysulfide-Based Foam with Hierarchical Pore Structure for Effective and Efficient Heavy Metal Sequestration

— Lawrence A. Limjuco, Rosemarie Ann I. Cuevas, Khino J. Parohinog, Grace M. Nisola, Wook-Jin Chung

Paper 562o: Development of Adsorbent Based on Layered Double Hydroxides Structure with High Mg/Al Ratio for Heavy Metal Removal

— **Byungho Kim**, Ki Bong Lee

Paper 562p: Characteristics of Heat Transfer in Carbon Dioxide Methanation Process

— **Doyeon Lee**, Myungwon Seo, Ho-Jung Ryu, Hyungseok Nam, Byung Wook Hwang, Kang Seok Go

Paper 562q: Development of a Biofilm-Based Technology for the Treatment of High Saline Process Wastewater

— Christian Tewinkel, Georg Fieg

Paper 562r: Synthesis of Fluorinated Hydrocarbon Anion Exchange Resins for the Removal of Perfluorinated Chemicals

— **Rob Spilker, Emily Kuehl**, Abby Smith, Hannah Wourms, Jason A. Berberich, Neil Danielson Paper 562s: Hybrid Technology for Soil Remediation: Foam Injection and Bioremediation

— Tomás-Eduardo Chávez-Miyauchi, Alejandro Islas-García, Anabelle Cerón-Nava, **María-Fernanda Flores-Súchil, María-Fernanda Ramírez-Pérez**

Paper 562t: Operational Experience of 0.5 Mwth Pressurized Chemical Looping Combustion System for Inherent CO₂ Separation

— Ho-Jung Ryu, Hyungseok, Nam, **Doyeon Lee**, Sung-Ho Jo, Seung-Yong Lee

Paper 562u: Pulsed Electric Field (PEF) Device Equipped with a Cathode Decorated with Copper-Titania Nanostructures for Enhanced Water Denitrification

— **Trixie Ruth N. Dy**, Jiayu Song, King Lun Yeung

Paper 562v: High-Intensity Narrow-Wavelength (Hi-NW) Light-Based Technology for Disinfection of MDRO in Environment

— **Ning Zhan, Jiayu Song**, King Lun Yeung

Paper 562w: Bacteriophage Recovery from Environmental Samples Using Functionalized Silica

— **Charlimagne Montealegre**, Wei Han, King Lun Yeung

Paper 562x: New Insights of Carbon Chain Length in Cross-Linked PEI Adsorbents on CO₂ Capture

— **Sunbin Jeon**, Ki Bong Lee

Paper 562y: Theoretical Modelling and Experimental Validation of Neutralization Reaction of Acidic Spillover By Calcium Hydroxide [Ca(OH),] and Sodium Bicarbonate [NaHCO,]

— **Hyunwook Jung**, Beyong-Hwan Ryu, Byungchan Han

Paper 562z: Simultaneous
Transformation of Hexavalent Chromium
and Carbon Tetrachloride Using
Atomized Zerovalent Iron in CoContaminant Aqueous Medium

— **Aadarsh Shah**, Ramesh Chawla, Brady Lee

Paper 562aa: Quantifying Regional Impacts to Atmospheric Nitrogen Deposition

— Sharmin Akter**, Kristina Wagstrom**

Paper 562ab: Cr(VI) Reduction By Fe(II) and Subsequent Regeneration of Fe(II) from Fe(III) By Shewanella Oneidensis MR-1

— **Md Alamgir Hossain**, Ramesh Chawla, Brady Lee

Paper 562ac: Magnetically Recoverable Carbon-Coated Iron Carbide for Organic and Arsenic Adsorptive Removal

— Camilah Powell, Sujin Guo, Lea M. Godret-Miertschin, Karen Ventura, Amanda W. Lounsbury, Dino Villagran, Julie B. Zimmerman, Ariel J. Atkinson, Paul Westerhoff, Michael S. Wong Paper 562ad: Biological Transformation of Hexavalent Chromium and Carbon Tetrachloride in Aqueous Medium By Shewanella Oneidensis Strain MR, and Cellulomonas Strain ES,

— **Michelle Cole**, Ramesh Chawla, Brady Lee

Paper 562ae: An Excel Tool for Economic and Environmental Analysis of Waste-to-Energy Technologies Processing Urban and Rural Waste

— **Olusola Johnson**, Daniela Cerna, John Kuhn, Babu Joseph

Paper 562af: Enhancing Nitroarene Reduction with Magnetically Recoverable AuFe Nanoparticles and Localized Heating Produced By an Alternating Magnetic Field (AMF) — Camilah Powell, Welman C. Elias,

Sujin Guo, Yiyuan Yin, Michael S. Wong
Paper 562ah: Removal of Heavy Metals

Paper 562ah: Removal of Heavy Metals from Contaminated Waters By Insoluble CMC Bio-Polymer

— Iman Nazari, Milad Vaezi

Paper 562ai: Thermal Treatment of the Aqueous Phase Resulting from the Hydrothermal Liquefaction of the Microalga *Chlorella vulgaris*

— **Johan A. Pasos**, Rubén Darío Godoy-Silva

Paper 562aj: Treating Liquid Effluents from Anaerobic Digestion: Semi-Empirical Modelling of a Multi-Stage Flash Evaporator

- Marek Vondra, Michal Touš

Paper 562ak: Pig Slurry Detoxication and Usage

— **Peter Letonja**, Tanja Weiß, Sarah A. Kunihs, Clemens Groß, Matthaeus Siebenhofer

Paper 562al: Systematic Synthesis of Wastewater Treatment Networks Using the P-Graph Approach

— Kirti M. Yenkie, Jean Pimentel, Akos Orosz, Ferenc Friedler

Paper 562am: Innovative Water Recycle Strategies for Reducing Water and Energy Use in Pulp and Paper Industry

— **Amod Parkhi**, Selen Cremaschi, Zhihua Jiang

Paper 562an: The Synergistic Emulsification of Cactus Mucilage with d-Limonene and Silica Nanoparticles for Oil in Water Emulsion

— **Fei Guo**, Zeinab Veisi, Norma Alcantar

Paper 562ao: Selective Oxygen
Reduction Using Methane for CO₂
Purification from a Simulated Flue Gas
— Andrew Kuhn, Zhitao Chen, Young

— Andrew Kuhn, Zhitao Chen, Yongqi Lu, Hong Yang

Paper 562ap: Modeling Chemical Absorption of CO₂ in Highly Alkaline Solutions for Direct Air Carbon Capture Applications

— Maria Camila Caceres Falla, Hector De la Hoz Siegler Jr. Paper 562aq: Pore Scale Investigation of CO₂ Storage and Bioconversion in Deep Saline Aquifers Using High Pressure Micromodels

— Anais Cario, Olivier Nguyen, Carole Lecoutre, Dominique Bernard, Yves Garrabos, **Samuel Marre**

Paper 562ar: Energy-Efficient Thermal Regeneration of Biphasic Solvents in a Laboratory CO₂ Desorption System — Qing Ye, Hong Lu, Hafiz Salih, Abiodun Oki, Paul Nielsen, Yongqi Lu

Paper 562as: Feasibility of Polyethylenimine-Based Silica Sorbent for Post-Combustion CO₂ Separation — Yao Ma, Vishnu Sriram, Joo-Youp Lee

Paper 562at: Physico-Chemical Activation of Biochar Using Acoustic Treatment and Amine Functionalization for Efficient CO, Adsorption

— **Riya Chatterjee**, Baharak Sajjadi, Wei-Yin Chen, Daniell Mattern

Paper 562au: Wastewater Treatment By Catalytic Wet Air Oxidation Process Based on Response Surface Methodology

— **Ghanim M. Alwan Sr.**, Mohamaad Abid. Lamvaa Abdul-Ridha

Paper 562av: Application of Ann and RSM Techniques in Optimal Parameter Evaluation for the Coag-Flocculation of Abattoir Effluent Using Crabshell Chitin — Paschal Ohale

Paper 562ax: Magnetic Graphene Oxide Modified with Chitosan and Cysteine Catalyst Was Synthesized for Removing (Pb 2+) lons from Aqueous Solution

— **Bizhan Honarvar**, Masoomeh Emadi

Paper 562ay: Degradation of N-Containing Pollutants By a Fenton-like Reaction with Cu-Based Catalysts

 Yang Sun, Yiyi Sheng, Doudou Ding, Pengfei Tian, Jing Xu, Yi-Fan Han
 Paper 562az: Modeling and Kinetics Study of Methyl Orange Degradation

over a Cu/y-Al₂O₂ Fenton-like Catalyst in

Continuous Fixed Bed Reactor

— Doudou Ding, Pengfei Tian, Yang
Sun, Jing Xu, Yi-Fan Han

Paper 562bb: Small-Pilot Plant for Tertiary Treatment of Domestic Wastewater Using Algal Photo-Bioreactor, with Artificial Intelligence — Ahmed Karam, Mohamed K. Mostafa, Abdelsalam Elawwad, Khaled Zaher, Ahmed S. Mahmoud, Robert W.

Paper 562bc: In Situ Treatment of Cyanotoxins in Water Sources Using Fiber-Immobilized TiO₂/Fe Nanoparticle Catalysts

— Suzana Ivandic

Paper 562bd: Degradation of Pharmaceutical Compound Diclofenac in Aqueous Solution By Horizontal Continuous-Flow Dielectric Barrier Discharge

— Yinhai Yang, Lecheng Lei, Bin Yang

Paper 562be: Green Oxidation Processes for Industrial Wastewater Treatments

— **Yang Kun-Lin**, Wing Fat Ho

Paper 562bf: Insights into the Properties of AgBiO₃ Photocatalyst and Its Application in Immobilized State for *E. coli* and 4-Nitrophenol Degradation — *Bhanupriya Boruah*, *Rimzhim Gupta, Jayant Modak, Giridhar Madras*

Paper 562bg: Experimental Study on the Removal of Polycyclic Aromatic Hydrocarbons Contaminants from Surface Water

— **Jian Fang**, Balaji Rao, Kayleigh Millerick, Renzun Zhao, Helen Lou, Danny Reible

Paper 562bh: Kinetics and Equilibrium Study of New Activated Carbon Materials for Acetaldehyde Removal — Simão P. Cardoso, Inês S.S. Ferreira, Inês Matos, Maria Bernardo, Marcia Ventura, Isabel M. Fonseca, Anabela Valente, Carlos M. Silva

Paper 562bi: The use of a new Fe Substituted Niobium Silicate (NS₉₁) for Hg(II) ion exchange from aqueous solutions

— **Simão P. Cardoso**, Zhi Lin, Elaine Fabre, Eduarda Pereira, Carlos M. Silva

Paper 562bj: Sustainable Strategies to Recycle Waste Electrical and Electronic Plastics by Thermochemical Processes

— **Pallab Das**, Jean-Baptise Sirven, Jean Chrispophe, Agnes Granjean, Dalton Tay, Jong-Min Lee

(563) Poster Session: Fuels and Petrochemicals Division

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Chau-Chyun Chen, Chair Paul M. Mathias, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

Paper 563b: The Influence of Ammonia on Flame Characteristics and Soot Formation in Ammonia/Methane Diffusion Flames

— **Matthew Montgomery**, Hyunguk Kwon, Yuan Xuan, Lisa Pfefferle, Charles S. McEnally

Paper 563c: Evaluation of Para- and Ortho-Xylene Adsorption on Beta Zeolite Using the Headspace Chromatography — F. Murilo T. Luna, Célio L. Cavalcante Jr, Jose Wilson Lima

Paper 563d: Study of the Influence of Antifoaming Additives on the Crude Oil/ Air Interface By Rheology

— **Mariana Mendes**, João B. V. S. Ramalho, Osvaldo Karnitz Jr., Luiz Carlos Palermo, Claudia E. Mansur

Paper 563e: Experimental and Theoretical Study of Viscosity Behavior of Sulfonated Partially Hydrolyzed Polyacrylamides (S-HPAM) with Long-Term Thermal Stability

— Xiaona Hu, Zhuo Yi, Xi Liu, Lunyu Zhu, Zhao Fang, Jinbiao Yang, Yajing Li Paper 563k: Extractive Denitrogenation and Desulfurization of Crude Oil Using Deep Eutectic Solvents

— **Samah E. E. Warrag, Ahmed Darwish**, Enas Al Nashef, Maaike C.
Kroon

Paper 563j: Processing Brazilian Presalt Crudes

— Gabriel Silva Pires de Almeida, Maria Elizabeth Pereira Leonel Marsialia

Paper 563f: Electrochemical Characterization of $SrTi_{0.3}Fe_{0.7}O_3$ - Δ -GDC Composite Anodes for Solid Oxide Fuel Cell

— **Xiaoyang Chen**, Qin Zhong, Tenglong Zhu

Paper 563I: Ceria-Lanthanide-Silver Oxides for Solar Thermochemical Conversion of CO₂

— Gorakshnath Takalkar, **Rahul Bhosale**, Suliman Rashid

Paper 563g: Advanced Optical Fiber Probe Technique to Measure Local Liquid Saturation and Velocity within Various Commercial Catalyst Shapes in Pilot Plant Trickle Bed Reactors (TBRs)

— Mohammed Al-ani, Muthanna H. Al-Dahhan

Paper 563h: Refinery Vacuum Ejector Systems: A Process Engineer's Perspective

- Andrew W. Sloley

Paper 563i: Influence of Long Time on Stream (TOS) in the Morphological and Structural Characteristics of Iron-Based Catalyst during FTS. A Closer Look at the Deactivation Routes

— Joshua Gorimbo

(564) Poster Session: Process Development

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S Joe Schroer, Chair Tony Wu, Co-Chair

Sponsored by: Process Development Division

Paper 564a: Immobilisation of Eosin Y on Wool for the Photocatalytic Synthesis of Fine Organic Chemicals

— Alba Acevedo Fernandez, Aneesa J Al-Ani, Duncan L. Browne, David R. Carbery, Emma Emanuelsson

Paper 564b: Towards Sustainable Industries: Industrial Symbiosis of an Oil Refinery and a Petrochemical Plant

— **Elham Ketabchi**, Evgenia Mechleri, Harvey Arellano-Garcia

Paper 564c: Selection of Isolation Methods for Micron Sized Particles — Mrunmayi D. Kumbhalkar, Wu Chen, Lin Zhao

Paper 564d: Techno-Economic Assessment of Hydrogen Production from Parallel Design Configuration of Fossil Fuel Derived Syngas Generation Processes

— Usama Ahmed

Paper 564e: Process Intensification of Biogas to Liquid (BGTL) Processes: A Techno-Economic Study

— **Benard Nyawanga**, Ahmed Naqi, Babu Joseph, John N. Kuhn

Paper 564f: Life Cycle Analysis of the Implementation of CO₂ Capture Process in Power Plants: Effect of Type of Fuel and Energy Demand

— Carolina Mora-Morales, Juan Pablo Chargoy-Amador, Eduardo Sanchez-Ramirez, Nelly Ramírez-Corona, Juan Gabriel Segovia-Hernández

Paper 564g: Systematic Design of Carbon Constrained Industrial Parks — *Dhabia Al-Mohannadi*

Paper 564h: CFD Study of Water Spray Cooling System for Refinery Process — Jiwon Roh, Il Moon, Man Sig Lee, Junghwan Kim

Paper 564i: Modelling of Anaerobic Digestion of Wastes from Industrial Processes

— **Pooja Sharma**, Uttam Kumar Ghosh, Amiya Kumar Ray

(565) Poster Session: Sustainability and Sustainable Biorefineries

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Ashley M. Pennington, Chair Christopher D. Dobrzanski, Co-Chair

Sponsored by: Sustainable Biorefineries

Paper 745f: Multi-Period Optimization Approach to Ocean Thermal Energy Conversion Systems for Closed Power Cycle — Ilse María Hernández-Romero, Fabricio Nápoles-Rivera, Luis Fabian Fuentes-Cortes, Antonio Flores-Tlacuahuac

BIOENERGY

Paper 565a: Relating Lignin Source and Processing History to Solubility in Diverse Solvents

— Villő E. Bécsy-Jakab, David Hodge

Paper 565b: Mechanical Properties and Bulk Flow Characterization of Loblolly Pine.

— Tiasha Bhattacharjee, Jordan Klinger, Tyler L. Westover, Aaron D. Wilson, Yidong Xia, Wencheng Jin, Hai Huang

Paper 565c: Production of (Bio) Butanol by Means of a Design for Sustainability Methodology

— Jessica Sanchez-Ramirez, David Vargas-Lopez, Lilia Arteaga-Espinoza, **Edgar Ramirez-Jimenez**

Paper 565d: Metabolic Response of Saccharomyces Cerevisiae and Clostridium Saccharobutylicum to Carbonyl Inhibition

— Yu Zhang, Maobing Tu

ATMOSPHERIC SCIENCE

Paper 565e: Site-Specific Covalent Immobilization of β-Agarase Onto Magnetic Nanoparticles for the Conversion of Gelidium Amansii into Biologically-Active Sugars

— Teklebrahan G. K. Weldemhret, Grace M. Nisola, Kristine Rose M. Ramos, Kris Niño G. Valdehuesa, Won-Keun Lee, Wook-Jin Chung

Paper 565f: Kinetic Studies on the CO₂ Gasification of Biochar for Use with SOFCs As a Bioenergy with Carbon Capture and Sequestration (BECCS) Process

— Derek Ni, Amanda Simson

Paper 565g: Role of Oxalate in Metal Separation and Recovery

— **Ankit Verma**, Rajkumar Kore, David R. Corbin, Mark B. Shiflett

Paper 565h: Evaluating Variability of Energy Consumption and Carbon Emissions of Activated Carbon Production from Wood Using Artificial Neural Network Integrated Process Simulations

— **Mochen Liao**, Steve Kelley, Yuan Yao

CLEAN AND SUSTAINABLE METHODOLOGY

Paper 565j: Well to Wake Analysis of Switchgrass to Butanol via Co-Fermentation of Sugar and Gas with Subsequent Conversion to Jet Fuel

— Abhiram Pamula, David J. Lampert, Hasan K. Atiyeh

Paper 565k: Novel Approach for Weighting in Geographic Information System Focused on a Multi-Stakeholder Problem- Case for Residual Biomass Processing System

— José Ezequiel Santibañez Aguilar, Diego Fabián Lozano-García, Antonio Flores-Tlacuahuac, Francisco José Lozano

Paper 565I: Quantifying Variability in Life Cycle Environmental Footprints of Bio-fuel Produced from Forest Residues in the United States

— Kai Lan, Longwen Ou, Stephen S. Kelley, Sunkyu Park, Hoyoung Kwon, Hao Cai, Michael Wang, Yuan Yao

(566) Poster Session: Transport and Energy Processes

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom R/S

Ryan Anderson, Co-Chair

Sponsored by: Transport and Energy

■ TRANSPORT PHENOMENA -EXPERIMENTAL AND NUMERICAL

Paper 566a: Wax Deposition in Subsea
Oil Transportation Pipelines

— Yingda Lu

Paper 566b: Characteristics of Phase Changing Material Nanoemulsions — Dinesh V. Kalaga, Robert J. Messinger, Artur Zych, Masahiro Kawaji Paper 566c: Evaluation of the Impact of Uncertainties of Measurement of Process Parameters in the Calculation of Incrustation Resistance in Crude Oil Heating Heat Exchangers

— Antônio Rimaci Miguel Junior, Fernando Luiz Pellegrini Pessoa, Ewerton Emmanuel da Silva Calixto, Fernanda Torres Paiva

Paper 566d: Hydrodynamics and Mass Transfer of Gas-Liquid Flow in a Tree-Shaped Parallel Microchannel with T-Type Bifurcations

— **Rongwei Guo**, Daofan Ma, Taotao Fu, Chunying Zhu, Xiqun Gao, Youguang Ma

Paper 566e: Modeling and Experimental Study on CO₂ Adsorption in Fixed-Bed Columns: Applications to Carbon Capture and Utilization

— Ram R. Ratnakar, **Santhosh Shankar**, Ravindra Agrawal, Birol Dindoruk

Paper 566f: Thermal Diffusion in Thermogalvanic Cells Containing Polymer Electrolyte

— **Daniel Hallinan Jr.**, Jesufane Mentor, Bryana Beckford

SYSTEM LEVEL ANALYSIS IN TEP

Paper 566g: Energy Optimization By Installation of Heat Recovery Steam Generator at Exhaust Gases of Gas Turbine Driven Compressor

- Kashif Jameel, Usman Asif

Paper 566h: Thermoenergetic Analysis of a Steam Generation and Distribution System

— Daniel Buendia Sr., Rivel Acevedo Sr.

Paper 566i: A Systematic Approach in Developing Alkaline Electrolysis Based Power to Gas Infrastructures Business Models

— **Jun-Hyung Ryu**, J. Jay Liu, Hankwon Lim

Paper 566j: Design of Optimized Carbon Dioxide Distribution Networks — *Muhamad Fariz Failaka*.

Muhammad Fahmi, Seno Prasetyo, Ali Elkamel

(567) 3D Printing Fundamental and Applications

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 28 Michael J. Bortner, Chair Richard Lakerveld, Co-Chair

Sponsored by: 3D Printing

3:30 Introductory Remarks

3:35 Paper 567a: 3D Printed Static Mixers for Continuous Reactive Crystallization

— **Kiran Mathew Thomas**, Richard Lakerveld

3:55 Paper 567b: Ultra-Low-Cost Continuous Manufacturing Platforms through 3D Printing and Telescoped Isolation Free Purification

— **Matthew Harding**, Rafael Lopez-Rodriguez, Sarah Brady, Denis Dowling, Kevin Girard, Steven Ferguson **4:15** Paper **567c**: Modeling of Poly(ether imide) in Material Extrusion Additive Manufacturing

— **Eric L. Gilmer**, David Anderegg, John M. Gardner, Emilie J. Siochi, David Dillard, Michael J. Bortner

4:35 Paper 567d: Harnessing a High Energy, Superconducting Electron Beam for Additive and Far-from-Equilibrium Manufacturing

— **Ryan D. Reeves**, Adam Duzik, Justin J. Hill

4:55 Paper 567e: Printing Hydrogels with Living Bacterial Cultures for Use As Chemical Bioreactors

— Jason Zeng, James Wilking

5:15 Paper **567f**: Characterization of Spatial Variability in Material Properties in Echogenically-Segmented Metal Components Fabricated By Additive Manufacturing

— **Kenneth Walton**, Manish Roy, Mikhail Skliar

5:35 Paper 567g: Lab Enablement through 3D Printing - Nitrogen Inertion Funnel

— Matthew Hagan

5:55 Concluding Remarks

(568) Additive Manufacturing of Energetics

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 21 Lori J. Groven, Chair Brandon Ennis, Co-Chair

Sponsored by: Energetics

3:30 Introductory Remarks

3:35 Paper 568a: Formulation of UV Curable Resins Utilized in Vat Photo Polymerization for the Additive Manufacturing of Gun Propulsion Charge in 3D Printers

— David Bird

3:55 Paper 568b: Viscoelastic Properties of Energetic Material Filled UV Photo Polymer Resins and Thermoplastic Feed Stock for the Additive Manufacturing of Gun Propulsion Charges

- Robin Crownover

4:15 Paper 568c: Development of a Vat Photo Polymerization 3D Printer for the Additive Manufacturing of Gun Propulsion Charge

— Elbert Caravaca

4:35 Paper **568d:** MgB₂/Fluoropolymer Filament and Pyrolant Combustion Studies

— Lance Kotter, Lori Groven

4:55 Paper 568e: Spherical Composite Powders As Feedstock for Additive Manufacturing

— **Daniel Hastings**, Edward Dreizin, Mirko Schoenitz

5:15 Paper 568f: Solids Metrics for Successful 3D Printing of Energetic Feedstocks

— Brandon Ennis, Naseem Jibrin, Benjamin Ennis, Michael Winn, **Bryan J. Ennis**

(569) Antifouling Membranes for Water Purification

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Peacock Spring

Jeffrey McCutcheon, Co-Chair Siamak Nejati, Co-Chair Seetha Manickam, Co-Chair

Sponsored by: Membrane-Based Separations

3:30 Paper 569a: Bio-Inspired Immobilization of Casein-Coated Silver Nanoparticles on Cellulose Acetate Ultrafiltration Membranes: From Laboratory to Scale-up

— **Xiaobo Dong**, Halle Shannon, Tequila Harris, Isabel Escobar

3:51 Paper 569b: Fouling Resistant Ultrafiltration Membranes with Ultrathin Hydrogel Selective Layers Containing Zwitterionic Moieties

— **Alice Aguiar**, Timothy Gronet, Ilin Sadeghi, Ayse Asatekin

4:12 Paper 569c: Zwitterion-Ag Complexes That Simultaneously Enhance Biofouling Resistance and Silver Binding Capability of Thin Film Composite Membranes

— *Ming Yi*, *Yan Wang*

4:33 Paper 569d: Fabrication of Fouling-Resistant Electro-Conductive Thin Film Composite Membranes By

Laminating Polyaniline (PANI) and

Reduced Graphene Oxide (rGO) on Polyethersulfone

— **Amin Karkooti**, Masoud Rastgar, Mohtada Sadrzadeh, Neda Nazemifard

4:54 Paper 569e: Development of Graphene Oxide-Coated Polyethersulfone Hollow Fiber Membranes with Improved Antifouling Property

- Preety Kumari, Jayesh R. Bellare

5:15 Paper 569f: Nanostructured Layer-By-Layer (LbL) Surface Modification of Nanofiltration Membranes for Effluent Treatment — *Oishi Sanyal, Wei Liao, Ilsoon Lee*

5:36 Paper **569g:** Molecular Drilling and Bonding for Highly Permeable and Fouling-Resistant Reverse Osmosis

— Yu Zhang, **Sui Zhang**

(570) Bioprinting of Scaffolds, Tissues, and Organs

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 12/13

Murat Guvendiren, Chair Xiaoyang Xu, Co-Chair Brian Aguado, Co-Chair

Sponsored by: Biomaterials

3:30 Paper 570a: Rapid Microfluidic Production of Cell-Laden Hydrogel Microspheroids

— Yuan Tian, Wen J. Seeto, Shantanu Pradhan, Petra Kerscher, **Elizabeth Lipke** **3:48** Paper **570b**: 3D-Printed PLLA-Peg-PLLA Nerve Guidance Channels for Peripheral Nerve Repair

— **Yang Hu**, Robert Newman, Adam Ekenseair

4:06 Paper 570c: Vascularized Multi-Tissue Platform – 3D Bioprinting an Organ Model *in Vitro*

— **Martin L Tomov**, Andrea Theus, Alex Cetnar, Holly Bauser-Heaton, Vahid Serpooshan

4:24 Paper 570d: Bioprinting Vascularized Cancer Models
— *Shen Ji, Murat Guvendiren*

4:42 Paper 570e: Chaotic Printing: Using Chaos to Fabricate Densely Packed Micro- and Nanostructure at High Resolution and Speed

— Grissel Trujillo-de Santiago, Carolina Chávez-Madero, Maria Diaz de Leon-Derby, Mohamadmahdi Samandari, Christian Carlos Mendoza-Buenrostro, Gyan Prakash, Carlos Fernando Ceballos-González, Juan Felipe Yee-de León, Ciro Angel Rodríguez-González, Y. Shrike Zhang, Mario Moisés Álvarez

5:00 Paper 570f: 3D-Bioprinting of Spatially Organized Bacterial Microcosmoi Using Chaotic Flows

— Carlos Fernando Ceballos-González, Carolina Chávez-Madero, Everardo González-González, Juan Felipe Yee-de León, Christian Carlos Mendoza-Buenrostro, Y. Shrike Zhang, Mario Moisés Álvarez, Grissel Trujillo-de Santiago

(571) CACHE 50th Anniversary: The Future of Cyber-Assisted Chemical Engineering Education

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom T

B. Wayne Bequette, ChairG. V. Rex Reklaitis, Co-Chair

Sponsored by: Miscellaneous

3:30 Paper 571a: Introduction
— G. V. Rex Reklaitis, B. Wayne
Bequette

3:35 Paper 571b: CACHE History

— Brice Carnahan, Warren D. Seider,
Larry Evans, Thomas F. Edgar

4:00 Paper 571c: CACHE Initiatives: Systems Biology

- Francis J. Doyle III

4:20 Paper 571d: CACHE Initiatives: Molecular Modeling

— Peter T. Cummings

4:40 Paper **571e:** CACHE Initiatives: Process Systems

— Richard Braatz

5:00 Paper **571f**: Beyond A -> B: Computational Approaches for Education in Reaction Engineering and Kinetics of Complex Systems

– Linda J. Broadbelt

5:20 Paper 571g: Graduate Research & Training in Molecular Data Science Through a University Wide Approach to Integrative Data Science Education — David Beck

5:40 Paper 571h: Survey: Computing in **Chemical Engineering**

- Martha A. Grover, Robert P. Hesketh

5:55 Wrap-up - G. V. Rex Reklaitis and B. Wayne Bequette

(572) Circulating Fluidized Beds Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 19 Allan Issangya, Chair Michael J. Molnar, Co-Chair

Sponsored by: Fluidization and Fluid-**Particle Systems**

3:30 Paper 572a: A Novel Circulating Fluidised Bed Solar Receiver Design for Thermal Energy Conversion and Storage — Mustapha Hamdan, Harvey Arellano-Garcia, Daniel Sebastia-Saez

3:50 Paper 572b: Performance of Different Types of Baffles Used in Gas-Solids Fluidized Bed Strippers

— **Allan Issangya**, S.B. Reddy Karri, T. M. Knowlton, Ben Freireich, Ray Cocco

4:10 Paper 572c: Dilute Phase Riser Dynamics – a Comparison of Scale - Ronald W. Breault, Steven Rowan, Jingsi Yang, Justin Weber

4:30 Paper 572d: CFD Simulation of Carbon Capture Using an Amine Based Solid Sorbent

— Farnaz Esmaeili Rad, Hamid Arastoopour, Javad Abbasian

4:50 Paper 572e: Coupled CFD-DEM Model of Fluidized Bed Drying of Pharmaceutical Wet Granules - Syed Ahsan, Bodhisattwa

Chaudhuri, Yijie Gao

5:10 Paper 572f: Numerical and Experimental Investigation of a Lab Scale Wurster Coating Process

— **Martina Trogrlic**, Thomas Forgber, Sharareh Salar-Behzadi, Avik Sarkar, Lourdes Contreras, Dalibor Jajcevic, Johannes G. Khinast

5:30 Paper 572q: 3D CPFD Simulation of Circulating Fluidized Bed Riser and Downer: Comparisons of Flow Structure and Solids Back-Mixing Behavior — Yancong Liu, Yingya Wu, Xiaogang

(573) Complex Fluids: Polymers and

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Orlando Ballroom M

Shi, Jinsen Gao, Xingying Lan

Macromolecules

Samanvaya Srivastava, Co-Chair Michelle A. Calabrese, Co-Chair

Sponsored by: Fluid Mechanics

3:30 Paper 573a: Pinch-Off Dynamics, Extensional Rheology, Foamability and Processability of Aqueous Solutions of Surfactant-Polymer Mixtures

— Carina Martinez, Jelena Dinic, Vivek Sharma

3:45 Paper 573b: Micro-Extensional Flow Behavior of Aqueous, Fibrillar Methylcellulose Solutions

- Athena E. Metaxas, Cari S. Dutcher

4:00 Paper 573c: Effects of Mesophase on Rheological Behavior of Pitch-Based Carbon Fiber Processing

- Heedong Yoon, Zachary R. Hinton, Nicolas J. Alvarez

4:15 Paper 573d: Distributions of Molecular Conformation in Flowing Solutions of Semidilute Polymers

Charles Young, Charles E. Sing

4:30 Paper 573e: Rheological Characterization of Polymer Networks and Heavily Entangled Polymer Melts Using Particle Rheology Simulations

- Pouria Nourian, Rafikul Islam, Nestor Valadez-Perez, Tsutomu Indei, Jay D. Schieber, Rajesh Khare

4:45 Paper 573f: Non-Homogeneous Flows of Entangled Polymer Solutions Driven By Flow-Concentration Coupling - Michael C. Burroughs, L. Gary Leal, Matthew E. Helgeson

5:00 Paper 573g: Microphase Separation in Entangled Polymeric Solutions

- Mohammad Hadi Nafar Sefiddashti, Brian J Edwards, Bamin Khomami

5:15 Paper 573h: The Effect of Harmonic Number on Large Amplitude Oscillatory Shear (LAOS) Testing of Starch Suspensions

— **Merve Yildirim Erturk**, Hazal Turasan, Jozef Kokini

5:30 Paper 573i: Critical-Layer Mechanisms in Elastoinertial Turbulence - Ashwin Shekar, Ryan McMullen, Suna-Nina Wana, Beverley McKeon, Michael D. Graham

5:45 Paper 573j: Direct Observation of Comb Polymer Dynamics in Semi-Dilute Solutions Using Single Molecule Imaging

— Charles M. Schroeder, Shivani F.

(574) Composites for Energy and **Environmental Applications**

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 11 Zhen Liu, Chair Han Lin, Co-Chair

Sponsored by: Composites

3:30 Paper 574a: Hierarchical "Nanoroll" like MoS,/Ti,C,Tx Hybrid with High Electrocatalytic Hydrogen **Evolution Activity**

- Jiapeng Liu, Yizhe Liu, Danyun Xu, Yuanzhi Zhu, Wenchao Peng, Yang Li, Fengbao Zhang, Xiaobin Fan

3:55 Break

4:20 Paper 574c: Copper-Carbon Nanomaterial Composite Coatings for Dramatic Improvements in Phase Change Heat Transfer

- Anju Gupta, Aniket Rishi

4:45 Paper 574d: Investigation of Coal Plastic Composite Materials As a Sustainable Building Material Alternative — **Jason Trembly**, Keerti

Kappagantula, Yahya Taha Ayed Al Majali, Clive Tafadzwa Chirume

5:10 Paper 574e: Colloidal, Nanoelectronic State Machines Based on 2D Materials As Smart Aerosolized Probes and Recorders

- Volodymyr Koman, Pingwei Liu, Daichi Kozawa, Albert Tianxiang Liu, Michael Strano

5:35 Paper 574f: Hexavalent Chromium Removal from Water Via Composite Nanofibers

- Yang Lu, Jesse Horne, Joshua Perch. Zhanhu Guo, Evan K. Wujcik

(575) Data Driven Optimization Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 26 **Ruth Misener, Chair** Masoud Soroush, Co-Chair

Sponsored by: Computers in **Operations and Information Processing**

3:30 Paper 575a: Sampling Domain Reduction for Surrogate Model Generation - Applied to Hydrogen Production with Carbon Capture — Julian Straus, Brage R. Knudsen,

Rahul Anantharaman

3:49 Paper 575b: Reduced Space Formulation for Global Optimization with Gaussian Processes (Kriging) Embedded - Artur M. Schweidtmann, Xiaopena Lin, Alexander Mitsos

4:08 Paper 575c: Bi-Level Mixed-Integer Optimization for Planning and Scheduling Integration Using the Domino Framework

- Burcu Beykal, Styliani Avraamidou, Efstratios N. Pistikopoulos

4:27 Paper 575d: Tuning with Hybrid Derivative-Free Optimization Initialization Strategies

- Benjamin Sauk, Nikolaos V.

4:46 Paper 575e: Data-Driven Branchand-Bound Algorithms for Optimization of Noisy Multi-Fidelity Simulation-Based **Problems**

— **Jianyuan Zhai**, Fani Boukouvala

5:05 Paper 575f: Optimization Algorithms for Dynamic Latent Variable **Problems**

- Sungho Shin, Alexander Smith, Joe Qin, Victor M. Zavala

5:24 Paper 575g: Reducing Computational Complexity of Integrated Scheduling and Control Using Machine Learning

- Calvin Tsay, Michael Baldea

5:43 Paper 575h: Evaluation of an MINLP Formulation for Symbolic Regression

— Marissa Engle, Nikolaos V. Sahinidis

(576) Design and Optimization of Environmentally Sustainable **Advanced Fossil Energy Systems** Wednesday, Nov 13, 3:30 PM

Hyatt Regency Orlando, Challenger 41/42

David C. Miller, Chair Michael S. Matuszewski, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

3:30 Paper 576a: Optimal Selection and Design of Energy Storage Technologies Integrated with Advanced **Energy Plants**

— Manali S. Zantye, Sai Pushpitha Vudata, Yifan Wang, Debangsu Bhattacharyya, M. M. Faruque Hasan

3:55 Paper 576b: Modular Gas-to-Liquids Process with Membrane Steam-Methane Reformer, Fischer-Tropsch Reactive Distillation and Integrated Product Refining

- Yu Xing, Sukmin Sung, Naien He, Cornelius Mduduzi Masuku, Lorenz T. Biegler

4:20 Paper 576c: Flexible Operation of CO, Capture Processes at Different Plant Scales

- **Mai Bui**, Niall Mac Dowell

Junghwan Kim

4:45 Paper 576d: A Novel Approach of Enhanced Gas Recovery Using Carbon Dioxide for Shale Gas Supply Chain Network in Unconventional Reservoirs - Yuchan Ahn, Joseph Sang-Il Kwon,

5:10 Paper 576e: Rigorous, Dynamic, Two-Film Model Development and Part-Load Optimization of a Solvent-Based CO₂ Capture Process Under Variable Capture Rate

- Paul Akula, John C. Eslick. Debangsu Bhattacharyya, David C.

5:35 Paper 576f: Integration of a Full-Scale Carbon Capture System with a 470-MW Lignite-Fired Power Plant

– Josh Stanislowski

(577) Development of **Pharmaceutical Process Control Strategies for Drug Substance** Manufacture

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 8 **Kevin Seibert, Chair** James C. Marek, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

3:30 Paper 577a: A Scale-Down and Feedback-Control Based Methodology to Optimize Multi-Step Extraction for Botanical Preparation on the Commercial Scale

— Fang Zhao, Haibin Qu

- **3:51 Paper 577b:** Scale-Independent Micronization: QbD Via a Specific Energy Model
- **Andrew DiPietro**, R. Rahn McKeown, David Rowe, Tara Jacklin, Samantha Rusk, Jessica Dixon
- **4:12** Paper 577c: A Comparative Study of Surrogate Model Based Control Strategy for a Pharmaceutical Crystallization Process
- Merve Öner, Kanjakha Pal, Frederico Montes, Stuart Michael Stocks, Jens Abildskov, Zoltan K. Nagy, Gürkan Sin
- **4:33 Paper 577d:** Specifications By Design: Framework for Setting Specifications to Maximize Flexibility and Meet Design Requirements
- **Shekhar K. Viswanath**, Shankar Vaidyaraman
- **4:54** Paper **577e**: Real-Time Concentration Monitoring Using a Compact Composite Sensor Array for Small-Scale Pharmaceutical Manufacturing Systems
- Mery Vet George De la Rosa, Rodolfo J. Romañach, **Torsten Stelzer**
- **5:15 Paper 577f:** Process Control Strategy for Synthetic Continuous Manufacturing
- Andrew J. Maloney, Elçin Içten-Gençer, XiaoXiang Zhu, Gerard Capellades, Matthew B. Beaver, Ayman Allian, Seth Huggins, Pablo Rolandi, Roger A. Hart, Shawn Walker, Richard D. Braatz
- **5:36** Paper **577g:** Industry 4.0: Advanced Bi-Layer Control System for Continuous Pharmaceutical Manufacturing Pilot-Plant
- **Ravendra Singh**, Rohit Ramachandran, Marianthi lerapetritou, Fernando J. Muzzio

(578) Developments in Extractive Separations: Processes

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Barrel Spring II George S. Goff, Chair Matthaeus Siebenhofer, Co-Chair

Sponsored by: Extractions

- **3:30** Paper **578a**: The Taylor-Couette Disc Contactor, a Novel and Flexible Apparatus for High Throughput Liquid-Liquid Extraction
- **Georg Rudelstorfer**, Annika Grafschafter, Matthaeus Siebenhofer
- **3:55 Paper 578b:** Heterogeneously Catalyzed Reactions with Solvent Extraction
- **Annika Grafschafter**, Tobias Maier, Georg Rudelstorfer, Matthaeus Siebenhofer
- **4:20 Paper 578c:** Cloud Point Temperature Purification of Butyric Acid from Aqueous Solutions Using Non-Ionic Surfactant
- **Remil Aguda**, Cody Stelly, William Holmes, Shayla LeBoeuf, Emmanuel Revellame

- **4:45 Paper 578d:** Continuous Micro-Extraction of Copper lons from Wastewater Using Ionic Liquids
- **Nahla Alamoodi**, Reyihangu Sulaiman, Inas M. Alnashef, Anas Alazzam
- **5:10** Paper **578e**: Evaluation of the Solvent Polarity on Extraction of Castor Oil By Soxhlet Method
- **José A. Pérez**, Marco F. Ortiz, Andrea C. Salas, Marley Vanegas
- **5:35 Paper 578f:** Solvent Extraction for Nanoparticle Purification
- Nopphon Weeranoppanant

(579) Directed and Self Assembly of Colloids

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom J Peter J. Beltramo, Chair Carlos Silvera Batista, Co-Chair

Sponsored by: Interfacial Phenomena

- **3:30** Paper **579a**: Estimation of Drying Length and Effect of Marangoni Flow during Particle Assembly By Convective Deposition
- Kedar Joshi, James F. Gilchrist
- **3:45 Paper 579b:** Overwriting Coffee-Ring Effect with Magnetostatic Convection
- **Jin Gyun Lee**, Vanel Porter, William A. Shelton Jr., Bhuvnesh Bharti
- **4:00 Paper 579c:** Sandwich Layering in Binary Colloidal Films through Autostratification
- Weiping Liu, Amanda Carr, Kevin Yager, Alexander F. Routh**, Surita Bhatia**
- **4:15 Paper 579d:** Vertically Aligning Ellipsoids with Electric Fields
- **Peter J. Beltramo**, Samuel Trevenen, John Klier
- **4:30 Paper 579e:** Complex Tessellations By the Sequential Assembly of Soft Colloids
- Miguel Angel Fernandez Rodriguez, **Fabio Grillo**, Maria-Nefeli Antonopuolou, Dominic Gerber, Lucio Isa
- **4:45 Paper 579f:** Designer Colloidal Matter
- **Hanumantha Rao Vutukuri**, Alfons van Blaaderen
- **5:00 Paper 579g:** Electric Field Mediated Interactions, Dynamics & Assembly of Superellipsoids
- Rachel Stein, Isaac Torres-Diaz, Michael A. Bevan
- **5:15 Paper 579h:** The Influence of Softness on the Stability of Binary Colloidal Crystals
- **R. Allen LaCour II**, Carl Simon Adorf, Julia Dshemuchadse, Sharon C. Glotzer
- **5:30** Paper **579i**: Colloidal Organization at Interfaces for Advanced Materials Applications
- Alismari Read, Sreeja Kutti Kandy, Iris B. Liu, Ravi Radhakrishnan, Kathleen Stebe

5:45 Paper **579**j: Controlled Electrochemical Deposition of Charge-Transfer Salt Nanorods on Nanoparticle Seeds — *Xuecheng Yu, Disni Gunasekara, Mohamed Kilani, Long Luo, Guangzhao Mao*

(580) Dynamic Processes at Interfaces

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom K Sepideh Razavi, Chair Susan Daniel, Co-Chair

Sponsored by: Interfacial Phenomena

- **3:30 Paper 580a:** Effect of Applied Potential on Friction between an AFM Probe and a Au(111) Surface
- Noshir Pesika
- **3:45** Paper 580b: Electroconvective Flow Mitigation through Viscoelastic Electrolyte Property Modifications *Alexander Warren*, *Lynden A*.
- **4:00** Paper **580c**: Frugal Lucas-Washburn Measurement of Microscale 3D Printing Powders Via Handheld Device
- **Katrina J. Donovan**, James Stasiak, Willie E. "Skip" Rochefort, Travis W. Walker
- **4:15** Paper 580d: Ultrafast Thin Liquid Film Spreading on Hierarchical Nanowire Superhydrophilic Surface Jiang Chun, Siyan Yang, Huiwen Yu, Tingting Hao, **Xuehu Ma**
- **4:30** Paper 580e: Interfacial Polymerization of a Thin Lubricious Film for Improving Wettability and Lubricity *Yifan Yu, Anuj Chauhan*
- **4:45** Paper **580f**: Interfacially Accelerated Micelle Destruction Promotes Enhanced Rates of Surfactant Adsorption
- **Joshua Mysona**, Alon McCormick, David Morse
- **5:00** Paper **580g:** Cholesterol Induced Morphological Transitions and Their Effect on Model Lung Surfactant Monolayer Rheology
- Cain Valtierrez-Gaytan, Ian Williams, Todd M. Squires, **Joseph A. Zasadzinski**
- **5:15** Paper 580h: Aggregation Propensities of Monoclonal Antibody Formulations Studied through Interfacial Behavior
- **Aadithya Kannan**, lan C. Shieh, Gerald G. Fuller
- **5:30** Paper **580i**: Quantifying the Competitive Adsorption between Monoclonal Antibodies and Surfactants at the Air/Water Interface Using X-Ray Reflectivity
- Ankit Kanthe, Mary Krause, Songyan Zheng, Andrew Ilott, Jinjiang Li, Wei Bu, Mrinal Bera, Binhua Lin, Charles Maldarelli, Raymond Tu

- **5:45 Paper 580j:** Interfacial Rheological Behavior of Janus Particles at the Air-Water Interface
- Luis E. Figueroa, Sepideh Razavi

(581) Electrochemical Advances to Enable Efficient Oxygen, Hydrogen and Water Reactions II

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom I Hong Yang, Chair Rachael H. Rothman, Co-Chair Gang Wu, Co-Chair

Sponsored by: Electrochemical Fundamentals

- **3:30** Paper **581a**: PEFC Electrode Layer Development Via Complementary *in Situ* Diagnostics and *Ex Situ* Characterization (invited)
- K.C. Neyerlin
- **3:52** Paper 581b: Formation of Carbon-Nitrogen Bonds in Carbon Monoxide Electroreduction (invited)
 — Feng Jiao
- **4:14** Paper 581c: Atomically Dispersed Metal Oxygen-Reduction Cathode Catalysts for PEM Fuel Cells *Gang Wu*
- **4:32** Paper **581d:** Ionic Liquid Interlayer for Enhanced Oxygen Reduction Reaction Electrocatalyst Activity and Durability
- **Joshua Snyder**, Yawei Li
- **4:50 Paper 581e:** The Role of the Sacrificial Metal Center in Promoting Electrocatalytic Activity in MOF-Based Catalysts
- **Talha Al-Zoubi**, Yu Zhou, Wei Gao, Charles E. Schulz, Hong Yang
- **5:08 Paper 581f:** Hydrogen Evolution Electrocatalysis with Core-Shell Ni-Mo @ Oxides
- **Rituja Patil**, Stephen House, Aayush Mantri, Judith C. Yang, James R. McKone
- **5:26 Paper 581g:** Co-Mo-TiO₂ Composite Electrocatalyst for the Hydrogen Evolution Reaction
 - **Cheng Wang**, Elizabeth J. Podlaha
- **5:44** Presentation

(582) Engineering the Tissue and Cell Microenvironment II: Disease Models and Mechanisms

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 2 Samira M. Azarin, Chair Tadas Kasputis, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30 Paper 582a:** Investigating Glioblastoma Stem Cell Behaviors in Three-Dimensional Hyaluronic Acid Hydrogels
- Pinaki Nakod, Yonghyun (John) Kim, **Shreyas Rao**

- **3:48** Paper 582b: Engineering a Novel Dynamic Multicellular Scaffold Based Model of Pancreatic Ductal Adenocarcinoma
- **Priyanka Gupta**, Paola Campagnolo, Andrew Nisbet, Roger Webb, Giuseppe Schettino**, Eirini Velliou**
- **4:06** Paper **582c**: High-Frequency Microrheology in 3D Reveals Mismatch between Cytoskeletal and Extracellular Matrix Mechanics
- **Woong Young So**, Jack R. Staunton, Colin D. Paul, Kandice Tanner
- **4:24** Paper **582d:** Stiffness Induces Metabolic Reprogramming in Primary Hepatocytes
- **Michael Moeller**, Senthilkumar Thulasingam, Srivatsan Kidambi
- **4:42 Paper 582e:** Characterizing the Irradiated Microenvironment with Normal Tissue Mammary Organoids
- **Benjamin C. Hacker**, Javier D. Gomez, Carlos Silvera Batista, Marjan Rafat
- **5:00** Paper **582f**: Targeting Hyaluronan Interactions for Glioblastoma Stem Cell Therapy
- Joline S. Hartheimer, Seungjo (Joe) Park, Shreyas Rao, **Yonghyun (John) Kim**
- **5:18** Paper **582g**: Invited: Designer Protein and Peptide Hydrogels As 3D Microenvironments for Neural Tissue Engineering
- Kyle Lampe

(583) Experimental Methods in Adsorption

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Blue Spring I/II Enzo Mangano, Chair Federico Brandani, Co-Chair

Sponsored by: Adsorption and Ion Exchange

- **3:30** Paper 583a: Digital Adsorption: 3D Imaging of Adsorption Equilibria and Dynamics in Technical Microporous Solids
- **Ronny Pini**, Lisa Joss, Sayed Alireza Hosseinzadeh Hejazi
- **3:50 Paper 583b:** Direct Characterisation of Gas Adsorption with Raman Spectroscopy
- **Kwanghee Jeong**, Arash Arami-Niya, Xiaoxian Yang, Gongkui Xiao, Gregor Lipinski, Markus Richter, Eric F. May, Paul L. Stanwix
- **4:10** Paper 583c: A New Technique to Measure Multicomponent Adsorption Equilibrium: Integral Mass Balance (IMB)
- **Orhan Talu**, Darren P. Broom, Michael J. Benham
- **4:30** Paper **583d**: A Combined Volumetric and FTIR Apparatus for the Measurement of Adsorption Kinetics *Luigi Canobbio, Giorgio Gatti,*

Leonardo Marchese, Stefano Brandani

- **4:50** Paper 583e: Use of a Novel Volumetric Differential Pressure Apparatus for Adsorption Equilibrium Measurements
- **Enzo Mangano**, Jinyu Wang, Stefano Brandani
- **5:10** Paper 583f: A New Method for Investigating Competitive Binary Adsorption Based on Nonlinear Frequency Response Analysis

Menka Petkovska

(584) Forum Plenary: Computational Molecular Science and Engineering Forum (Invited Talks)

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Rock Spring I/II Jim Pfaendtner, Chair Sapna Sarupria, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

- **3:30 Paper 584a:** Modeling the Preparation and Reactivity of Amorphous Catalysts
- **Baron Peters**, Craig Vandervelden, Salman Khan, Susannah L. Scott
- **4:10** Paper **584b**: Molecular Recognition of Ice By Proteins: From Ice Nucleation to Antifreeze
- Valeria Molinero
- **4:30 Paper 584c:** Too Small Is Never Too Small: Utilizing Advanced Path Sampling to Probe the Kinetics and Mechanism of Rare Events, from Atmospheric Ice Nucleation to Membrane Transport
- Amir Haji-Akbari
- **5:10** Paper **584d**: Combining Density Functional Theory Calculations with Machine Learning for Studying Complex Chemistries on Surfaces
- Andreas Heyden
- **5:30** Paper **584e:** Modeling Nucleation of Organic Molecules with the String Method
- Erik E. Santiso

(585) How We Teach: First Year Students Survey Results (Invited Talks)

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 23 Laura P. Ford, Chair Margot A. S. Vigeant, Co-Chair

Sponsored by: Undergraduate Education

- 3:30 Welcoming Remarks
- 3:35 Introductory Remarks
- **3:40** Invited Talk: Summary of Survey Results
- **4:10** Paper **585a:** Invited Talk: Purdue University's First-year Experience
- Isabel Jimenez-Useche
- 4:40 Discussion
- 5:25 Concluding Remarks

(586) Industry Perspectives on Membrane Separations (Invited Talks)

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Barrel Spring I Dhaval Bhandari, Co-Chair Nitesh Bhuwania, Co-Chair Haiqing Lin, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30 Paper 586a:** Commercializing a Membrane Technology in the Oil and Gas Industry
- Hannah Murnen
- **3:55 Paper 586b:** Major Applications of Osn Membrane Technology

 Kumar Abhinava
- **4:20 Paper 586c:** Membrane Based Acid Gas Separation: Past, Present and Future
- Ankur Jariwala
- **4:45 Paper 586d:** Onboard Fuel Separation
- Randall Partridge
- **5:10 Paper 586e:** Gas Separation Membrane Innovation at Air Liquide *Yong Ding*

(587) Integrated Process Engineering and Economic Analysis

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Regency Ballroom Q Yizu Zhu, Chair Julie N. Renner, Co-Chair Mike Dou, Co-Chair Jerry Kaczur, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

- $\bf 3:30$ Paper $\bf 587a:$ A Comparison of Two Bioconversion Processes for the Production of Commercially Important $\bf C_4$ Streams
- **Chinmay Satam**, Manuel Daub, Matthew J. Realff
- **3:42** Paper 587b: An Integrated Tool for Rapid Assessment of Chemical Manufacturing Process Emissions, Treatment and Sustainability Performance
- **Selorme Agbleze**, Shuyun Li, Gerardo J. Ruiz-Mercado, Fernando V. Lima
- **3:54 Paper 587c:** Exploring the Potential of Chemical Looping Systems to Provide Alternative H₂ Production Systems Solutions Using Process Simulations and Techno-Economic Analysis
- **Mandar Kathe**, Melanie Gross, Fanhe Kong, Deven Baser, William K. Wang, Peter Sandvik, L.-S. Fan
- **4:06** Paper 587d: Economic Analysis of Battery (NMC) Cathode Material Production in Flame Spray Process with Sustainable Solvents
- **Guiyan Zang**, Jianan Zhang, Siqi Xu, Yangchuan Xing

- **4:18** Paper **587e**: Soybean Oil As a Bio-Solvent to Sweeten Sour Natural Gas — *Emma C. Brace*, *Abigail S. Engelberth*
- **4:30** Paper 587f: Reducing Energy, Solvent, and Resin Demand of Sorption-Based Processes for Carboxylic Acid Recovery
- **Patrick Saboe**, Lorenz Manker, Hanna Monroe, William Michener, Stefan Haugen, Gregg T. Beckham, Eric M. Karp
- **4:42** Paper **587g**: Storage of Excess Wind Energy and Utilization of Waste Flue Gas ${\rm CO}_2$ through Sustainable Methanol Production
- Bjartur Máni Sigurðarson, Hsi Tsao, Ingrid Ammitzbøll Helgeland, Gürkan Sin
- **4:54 Paper 587h:** Towards a Novel Energy Financial Security: The Texas A & M Energy Spot Price Index
- **Stefanos G. Baratsas**, Alexander M. Niziolek, Onur Onel, Logan R. Matthews, Christodoulos A. Floudas, Detlef R. Hallermann, Sorin M. Sorescu, Efstratios N. Pistikopoulos
- **5:06** Paper **587i**: Techno-Economic Analysis of Septic Tank Waste Treatment in a Centralized Hydrothermal Treatment Facility
- **Kyle McGaughy**, Akbar Saba, Nepu Saha, M.Toufiq Reza
- **5:18** Paper **587**j: Turning a Hazard into Sustainable Revenue Streams: H₂S Valorization in Offshore Oil and Gas Productions through Process Intensification
- Abhimanyu Pudi, Vahid Shadravan, Louise la Cour Freiesleben, **Adam Karcz**, Martin Andersson, Seyed Soheil Mansouri
- **5:30 Paper 587k:** Critical CO₂ Carnot Engine for Industrial Waste Heat Recovery and Utilization
- Sarah Makuc, Eldred Chimowitz
- **5:42** Paper **587**I: Industrial Symbiosis at an Industrial Park in Trinidad and Tobago: A Focus on Carbon Dioxide *Thérèse G. Lee Chan, David A. Janes*

(588) KIChE-US Chapter Open Forum (Invited Talks)

Wednesday, Nov 13, 3:30 PM
Hyatt Regency Orlando, Celebration 10
Hyunmin Yi, Chair
Jin Ryoun Kim, Co-Chair
Hyun-Tae Hwang, Co-Chair

Sponsored by: International Committee

- **3:30 Paper 588a:** Shape Control of Monodispersed Block Copolymer Particles
- Bumjoon J. Kim
- **3:50** Paper **588b**: When Misbehaving Proteins Met Well-Behaved Proteins...

 Jin Ryoun Kim

- **4:10 Paper 588c:** Polymer Lung Surfactant Therapy for Respiratory Distress Syndrome
- You-Yeon Won
- **4:30 Paper 588d:** Additives Applied to Cu Electrodeposition
- Jae Jeong Kim
- **4:50** Paper **588e**: Multiscale Modeling of Pulp and Paper Manufacturing Process
- Joseph Sang-Il Kwon
- **5:10** Paper 588f: Tissue-Engineered Trabecular Bone Model Using Demineralized Bone Slices
- Jungwoo Lee
- **5:30 Paper 588g:** Infiltration of Polymers into Disordered Nanoparticle Packings: Polymers Under Extreme Nanoconfinement
- Daeyeon Lee

(589) LAAARGE Classroom Techniques

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 22 Daniel Knight, Chair Jason E. Bara, Co-Chair Troy Vogel, Co-Chair

Sponsored by: Undergraduate Education

- **3:30 Paper 589a:** Establishing a Learning Assistant (Peer Leader) Training Program
- Sandra L. Pettit, Molly Skinner
- **3:48** Paper **589b**: Student-Created Youtube Videos, a Multimedia Assignment, Improves Engaged Student Learning Outcomes in a Large Engineering Classroom
- **Andrew Zak**, Luke F. Bugada, Fei Wen
- **4:06 Paper 589c:** A Framework for Developing Concept Questions for Active Learning in Large Classes
- **Milo D. Koretsky**, Susan Nolen, Brian Self, Michael Prince
- 4:24 Paper 589d: Problem Solving When Using Student-Written Problems That Reverse-Engineer Youtube Videos Uchenna Asogwa, T Ryan Duckett, Amanda P. Malefyt, Gale Mentzer, Charlene Czerniak, Matthew Liberatore
- **4:42 Paper 589e:** Large Classes Create Big Data: Grades, Grading, and Grade Spreadsheets
- Matthew Liberatore
- **5:00** Paper **589f**: Approaches to Maintain Student Support on Projects with Increased Class Size

 Troy Vogel
- **5:18** Paper **589g**: Specifications Grading: Simplify and Save Time *Jennifer Pascal, Kristina Wagstrom*

(590) Mesoscale Modeling Advances for Thermodynamics, Transport and Reaction

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Silver Spring

Shuangliang Zhao, Chair Ning Yang, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **3:30 Paper 590a:** Bioinspired Construction and Performance Intensification of Photo-Enzyme Coupled Enzymatic System
- Jiafu Shi, **Zhongyi Jiang**
- **3:45 Paper 590b:** Mesoscale Simulation and Experimental Study on Supported Catalysts
- Jianguo Wang
- **4:00** Paper **590c:** Dynamic Adsorption of lons into like-Charged Nanoslits
- Leying Qing, Shuangliang Zhao
- **4:15** Paper **590d**: Prediction of Thermal Conductivity of Silicon Nanowires on Basis of High Performance Computing
 Chaofeng Hou
- **4:30 Paper 590e:** A Structure-Based Drag Model for Coarse-Grid Euler—Lagrange Simulations
- Yaxiong Yu, Qiang Zhou
- **4:45** Paper 590f: Reaction Density Functional Theory and Its Application to SN₂ and Nucleophilic Addition Reactions in Aqueous Solution
- **Cheng Cai**, Weiqiang Tang, Shuangliang Zhao, Honglai Liu
- **5:00 Paper 590g:** Quantifying Confinement Effects on Fluid Transport Via Multi-Scale Simulations
- Anh Phan, Dian Fan, Maria Apostolopoulou, Sakiru Badmos, Tran Le, **Alberto Striolo**
- **5:15** Paper **590h**: Modeling Reaction-Diffusion in Combustion Processes Using Smoothed Dissipative Particle Dynamics
- **Nikolai D. Petsev**, Xia Ma, Bryan Henson, Brad Clements
- **5:30 Paper 590i:** Mesoscopic Models for Electro-Hydrodynamic Interactions of Polyelectrolytes
- Shujun He, Ryan J. Montes, Jason E. Butler, **Dmitry I. Kopelevich**
- **5:45 Paper 590j:** Internal and External Soot Oxidation
- **Georgios A. Kelesidis**, Sotiris E. Pratsinis
- (591) Modeling, Control, and Optimization of Energy Systems Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 25 Alexander W. Dowling, Chair Luis A. Ricardez Sandoval, Co-Chair

Sponsored by: Systems and Process Control

- **3:30** Paper **591a**: Dynamic Timescale-Based Reduced Order Models for Simulating Moving Bed Chemical Looping Combustion Reactors
- **Robert Parker**, Lorenz T. Biegler
- **3:47 Paper 591b:** Modeling and Model Predictive Control of a Countercurrent Polymer-Based Water-Gas Shift Membrane Reactor for Process Intensification
- **Brent Bishop**, Yacine Feliachi, Xin He, Fernando V. Lima
- **4:04** Paper **591c:** A Hybrid Stochastic/ Gradient-Based Multi-Objective Dynamic Optimization of Vacuum Swing Adsorption
- **Zhimian Hao**, Artur M. Schweidtmann, Yannic Vaupel, Adrian Caspari, Alexei A. Lapkin, Adel Mhamdi, Alexander Mitsos
- **4:21 Paper 591d:** Optimization of Liquid Petroleum Products Pipeline Operations
- Elena Khlebnikova, Mary Ewers, Kaarthik Sundar, Anatoly Zlotnik, Byron Tasseff, Russell Bent
- 4:38 Paper 591e: Handling
 Microseismic Measurement Uncertainty
 in Fracture Geometry Control of
 Hydraulic Fracturing
 Prashanth Siddhamshetty, Joseph
- Sang-II Kwon
 4:55 Paper 591f: Uncertainty
- Mitigation Via Short-Term Rescheduling in Cascaded Hydropower Systems

 Pulkit Mathur, Christopher L. E.

Swartz, Danielle Zyngier, Francois Welt

- **5:12 Paper 591g:** Spatio-Temporal Modeling and Optimization of Energy Infrastructure Networks
- **Jordan Jalving**, Eric Tatara, Victor M. Zavala
- **5:29 Paper 591h:** The Role of Carbon Capture and Sequestration As a Resilient Technology in the UK's Electricity System Decarbonisation: A Techno-Economic Analysis for Energy Policy Design
- **Yoga Wienda Pratama**, Niall Mac Dowell

(592) Molecular Simulation of Adsorption II

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Manatee Spring II Gennady Gor, Chair

Daniel W. Siderius, Co-Chair

- **Sponsored by:** Adsorption and Ion Exchange
- **3:30 Paper 592a:** Nuclear Quantum Effects on Adsorption in Nanoporous Structures
- Abhishek Bagusetty, J. Karl Johnson

- **3:48** Paper **592b:** Toward Sustainable Metal-Organic Frameworks for Post-Combustion Carbon Capture Identifying Improvement Opportunities By Molecular Simulation and Life Cycle Assessment
- **Jingying Hu**, Li-Chiang Lin, Bhavik R. Bakshi
- **4:06** Paper **592c**: DFT Study for Developing Novel and Specific B₅-Type Step Site Scaling Relations and BEP Analysis for Stepped HCP Catalyst Surfaces
- Rees B. Rankin
- **4:24** Paper **592d:** Impact of H₂O and CO₂ on Methane Storage in Metal-Organic Frameworks
- Daniel Gonçalves, Randall Q. Snurr, **Sebastiao M. P. Lucena**
- **4:42** Paper **592**e: Predictive Models of Azeotropic Adsorption from Molecular Simulations and Macroscopic Theories *Roberto Mennitto*, *Lev Sarkisov*, *Stefano Brandani*
- **5:00** Paper **592f**: Density Functional Theory Study of Biomolecule Adsorption to Graphene and Modified Graphene: Molecular Insights into Biofilm Formation and Adhesion
- **Sourav Verma**, Kenneth M. Benjamin
- **5:18** Paper **592g**: Understanding the Adsorption of 4th Generation Refrigerants on Metal-Organic Frameworks By Molecular Simulations *Husam A. Al-Araj, Daniel*
- **Bahamon**, Ali A. Alnajjar, TieJun Zhang, Maryam Khaleel, Lourdes F. Vega
- **5:36** Paper **592h**: Modeling the Adsorption of Isobutane/Butene on Hydrophobicity/Hydrophilicity Modified Solid Acid Surface
- Piao Cao, Weizhong Zheng, Weizhen Sun, Ling Zhao

(593) Nanofabrication and Nanoscale Processing II

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Discovery 45 Jung-Sheng Wu, Chair Erick S. Vasquez, Co-Chair

Sponsored by: Nanoscale Science and Engineering Forum

- **3:30** Paper **593a**: Shape Memory Assisted Contact Printing in Nanoscience and Electronics *Alexander Shestopalov*
- **4:00** Paper **593b**: Vertically Aligned Boron Nitride Nanotube Composites for Thermal Conductivity Improvements *Kayla O'Neill, Justin J. Hill, Michael Cutbirth*
- 4:15 Paper 593c: Electrochemical Growth of Charge Transfer Complex Micro/Nanowires on Microelectrodes and Their Application in Gas Sensing — Mohamed Kilani, Disni Gunasekara, Xuecheng Yu, Long Luo, Guangzhao Mao

- **4:30** Paper **593d:** Series Flash Nanoprecipitation for the Scalable Formulation of Nanoparticles with Ultra-High (>90%wt) Core Loading for Imaging and Drug Delivery Applications
- **Leon Z. Wang**, Kurt D. Ristroph, Brian K. Wilson, Bryan J. Kudisch, Robert K. Prud'homme
- **4:45 Paper 593e:** Process Safety and Scale-up of Graphene Oxide Synthesis and Storage
- **Pritishma Lakhe**, Devon Kulhanek, Wanmei Sun, M. Sam Mannan, Micah I. Green
- **5:00** Paper **593f**: Laser Ablation Synthesis in Solution for the Rational Design of Hybrid Carbon-Based Nanocomposites for Enhancements in Electrochemical Storage and Conversion Systems
- **Erick L. Ribeiro**, Sheng Hu, Dibyendu Mukherjee, Bamin Khomami
- **5:15 Paper 593g:** Ultrasonic Assisted Self-Assembly of Polystyrene Nanospheres
- **Gloria Alvarado**, Alona Komarenko, Luis Manuel, Ali Mehrnezhad, Kidong Park, Kevin M. McPeak
- **5:30** Paper **593h**: Micro-Chemical Technology Tune Nanoscale Structure of Nanoparticles and Its Bioapplication *Mingwei Wang*
- **5:45 Paper 593i:** High Density Oxygen Storage in Nanometer Scale Deep Capillaries
- **Adam Duzik**, Gregory E. Chester, Ryan Reeves, Justin J. Hill

(594) Nanomaterials for Hydrogen Production and Fuel Cells II: Water-Splitting

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Discovery 46

Sponsored by: Nanomaterials for Energy Applications

- **3:30 Paper 594a:** First-Principles Computational and Machine Learning Approach to Innovative Design of Electrocatalysts
- Byungchan Han, Jeemin Hwang
- **4:00 Paper 594b:** Improving Precision in Materials Synthesis for Hydrogen Electrocatalysis
- **Rituja Patil**, Qiudi Meng, Thomas Allen, James R. McKone
- **4:20 Paper 594c:** Nanoscopic Control of the Interfaces to Optimize Metal-Insulator-Semiconductor Systems for Solar Water Splitting
- **John Hemmerling**, Joseph Quinn, Suljo Linic
- **4:40** Paper **594d:** Synthesis of Silica Supported Ni and Cu Catalyst for Carbon Dioxide Conversion
- **Ahmed Aheed**, Mohd Ali H Saleh Saad**, Anand Kumar**
- **5:00** Paper **594e**: Directed Self-Assembly of Block Copolymers for Well-Defined Nanostructured Electrocatalysts *Christopher G. Arges*, *Deepra*

Bhattacharya, Le Zhang

- **5:20** Paper **594f**: The Novel Electrocatalyst/Semiconductor Photoelectrodes for Efficient Photoelectrochemical Water Splitting *Xingwang Zhang*, *Lecheng Lei*, *Bin Yang*, *Zhongjian Li*
- **5:40** Paper **594g**: Biomineralized Metal Chalcogenide Quantum Dot/Rgo Photocatalysts for Water Splitting *John Sakizadeh, Joseph Cline, Mark Snyder, Christopher J Kiely,* **Steven**

(595) Nanoscale Structure in Polymers

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 14 Shudipto Konika Dishari, Chair Sangwoo Lee, Co-Chair

Sponsored by: Polymers

- **3:30 Paper 595a:** Multi-Scale Ordering in Highly Stretchable Polymer Semiconducting Films
- **Jie Xu**, Hung-Chin Wu, Zhenan Bao
- **3:47** Paper 595b: Impact of Helical Chain Shape in Sequence-Defined Polymers on Polypeptoid Block Copolymer Self-Assembly *Emily Davidson*
- **4:04 Paper 595c:** Combining Polymer Synthesis with Self-Assembly of Block Copolymers
- **Zhe Qiang**, Muzhou Wang
- **4:21** Paper **595d:** 3D Analysis of Nanostructured Polyamide Membranes Using Quantitative Electron Tomography
- Hyosung An, John W. Smith, Wenxiang Chen, Nestor J. Zaluzec, Matthew A. Kulzick, Qian Chen
- **4:38 Paper 595f:** Solvent Vapor Annealing to Control Polymer Crystal Morphology
- Samuel Bliesner, Julie N. L. Albert
- **4:55** Paper **595**g: Cation Conduction in Nanostructured Side-Chain Ionomers
- Jiacheng Liu**, Jennifer Schaefer**
- **5:12 Paper 595h:** Poly(ionic liquid) Pentablock Terpolymer Electrolytes in Solid-State Lithium Ion Batteries
- **Tzu-Ling Chen**, Rui Sun, Carl L. Willis, Yossef A. Elabd
- **5:29** Paper **595**i: Self-Assembly and Ion Transport of Hybrid Organic-Inorganic Diblock Copolymers with Salt *Nitash P. Balsara*, *Gurmukh Sethi, Irune Villaluenga*

(596) Nanostructured Thin Films Wednesday, Nov 13, 3:30 PM Hvatt Regency Orlando, Celebration 16

Hyatt Regency Orlando, Celebration 16 Seok-Jhin Kim, Chair Chen Zhang, Co-Chair

Sponsored by: Inorganic Materials

- **3:30 Paper 596a:** Development of a Functional Coating to Mitigate Coking in a Turbocharger Compressor
- Pallav Jani, Galen B. Fisher, John Hoard, Johannes W. Schwank, Giovanni Cavataio, Dairene Uy

3:48 Paper **596b**: Facile Fabrication of Lead Chalcogenide Thin Films with Controlled Structure and Composition — *Kyle Weideman*, *Swapnil Dattatray Deshmukh*, *Yining Feng*, *Na Lu*, *Rakesh*

Agrawal

- **4:06** Paper **596c**: Effects of Pore Size on Molecular Transport of Ionic Liquid ([BMIM][PF₆]) Confined in Nanoporous Silica Films
- **Yuxin He**, Folami Ladipo, Barbara L. Knutson, Stephen E. Rankin
- **4:24** Paper **596d**: Lithium Batteries Enabled By Robust Thin Film Composite Solid Electrolyte Separators
- Shaofei Wang, Marina M. Ioanniti, Wyatt Tenhaeff
- **4:42** Paper **596e**: Selective Atomic Layer Deposition of Zirconia on Electroplated Copper Substrates
- **Soumya Saha, Nickolas D Anderson**, Gregory Jursich, Christos G. Takoudis
- **5:00 Paper 596f:** Fabrication of Nanostructured Thin Films By ALD for Spacecraft Applications
- **Raymond A. Adomaitis**, Hossein Salami, Alan Uy, Aarathi Vadapalli, Brianna Sheard, Vivek Dwivedi
- **5:18** Paper 596g: Intermetallic Hydrogen Separation Membranes: Synthesis and in-Situ Characterization *Casey O'Brien*
- **5:36 Paper 596h:** Formation of Quantum Dots on Epitaxial Semiconductor Films Grown on Pit-Patterned Substrates
- **Chao-Shou Chen**, Ashish Kumar, Dimitrios Maroudas

(597) North American Mixing Forum Award Session (Invited Talk)

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 32 David S. Dickey, Chair Clara Gomez, Co-Chair Sujit Bhattacharya, Co-Chair

Sponsored by: North American Mixing Forum

- **3:30 Paper 597a:** On the Joint Use of Simulation and Experimentation to Clarify Solid-Liquid Mixing Behavior
- François Bertrand

(598) Novel Nanoparticles and Nanostructured Materials for Pharmaceuticals and Medical Applications

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 20 Georgios A. Sotiriou, Chair Timothy M. Brenza, Co-Chair

Sponsored by: Nanoparticles

- **3:30 Paper 598a:** Thermal Decomposition Synthesis of Monodisperse, Phase-Pure Iron Oxide Nanoparticles for Mpi and Magnetic Hyperthermia Applications
- **Shehaab Savliwala**, Sitong Liu, Carlos Rinaldi

- 3:50 Paper 598b: Magnetic Nanoparticle Clusters for Efficacious Bilirubin Removal from Body Fluids — Alexandre Anthis, Martin T. Matter, Kerda Keevend, Lukas R. H. Gerken, Inge K. Herrmann
- **4:10** Paper **598**c: Antioxidant Protection from Oxidative Stress Damage in Human Pulmonary Cells *Jordan A. Hoops, Timothy M. Brenza*
- **4:30 Paper 598d:** Crosslinking of Ovalbumin Nanoparticles Affects Cellular and Humoral Immune Responses
- Nahal Habibi, Stephanie Christau, Lukasz Ochyl, James Moon, Joerg Lahann
- **4:50 Paper 598e:** Encapsulation of Poorly Water-Soluble Drugs into Yeast Glucan Particles By Spray Drying: Improvement of Dispersion and Dissolution Properties
- **Gabriela Ruphuy Chan**, Ivan Saloň, Jan Tomas, Petra Šalamúnová, Jaroslav Hanuš, František Štěpánek
- **5:10** Paper **598f**: Multiscale Analysis of Topically Applied Nanoparticulate Adhesives: Biodistribution and Biotransformation
- **Martin T. Matter**, loana Lese, Inge K. Herrmann
- **5:30 Paper 598g:** Model for the Evolution of Gold Nanoparticles in the Citrate Synthesis Method
- **Emmanuel Agunloye**, Asterios Gavriilidis, Luca Mazzei

(599) Nucleation and Growth II Wednesday, Nov 13, 3:30 PM

Hyatt Regency Orlando, Manatee Spring I

Meenesh R. Singh, Chair Marina Tsianou, Co-Chair

Sponsored by: Crystallization and Evaporation

- **3:30** Welcoming Remarks
- **3:33 Paper 599a:** Prenucleation Motifs of Various Dimensionality in Entropic Crystallization
- **Sangmin Lee**, Erin G. Teich, Michael Engel, Sharon C. Glotzer
- **3:54** Paper **599b:** A Multidimensional Free Energy Approach for Polymorph Selection in Crystallization of Glycine from Solution
- **Pelin Su Bulutoglu**, Nandkishor Nere, Shailendra Bordawekar, Doraiswami Ramkrishna
- **4:15** Paper **599c**: Towards Digital Design of Crystals: Predicting Absolute Chemical Potentials for Solid, Solution and Gas Phases
- **Vikram Khanna**, Michael F. Doherty, Baron Peters
- **4:36 Paper 599d:** Irreversible Inhibition of Hematin Crystallization By Cooperative Phase Behaviors Induced By Antimalarials
- **Wenchuan Ma**, Peter Vekilov, Jeffrey D. Rimer

- **4:57** Paper **599e:** Identification of Polymorph Specific Molecular Interactions during the Process of Crystallization
- Anish V. Dighe, Meenesh R. Singh
- **5:18 Paper 599f:** When Crystals Don't Grow the Growth Dead Zone
- **Yumin Liu**, Aurora J. Cruz-Cabeza, Roger J. Davey
- **5:39 Paper 599g:** Crystallization of MIL-53 Metal Organic Frameworks (MOFs) through Changes in the Hydrothermal Process
- Andrew R. Garcia, Kirk J. Ziegler, Sergey Vasenkov
- (600) Particle Engineering and Crystallization in Materials Science Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 6 Anil Rane, Chair Steven J. Brenek, Co-Chair
- **Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum
- **3:30** Paper 600a: Avoiding Distribution Confusion: Using the Information in Particle Size Distributions
- **Jacob Albrecht**, John Gamble, Ana Ferreira, Mike Tobyn, David Good
- **3:55 Paper 600b:** Combining Liquid-Liquid Phase Separation and Mesoporous Carrier to Deliver Drug Product Intermediate
- **Moussa Boukerche**, Sean Garner, Nandkishor Nere
- **4:20 Paper 600c:** Optimising the Nucleation of Polypeptides Using Nanotemplates: The Case Study of Insulin
- Frederik J. Link, Jerry Y. Y. Heng
- **4:45** Paper 600d: Surface-Induced Nucleation Strategies: Seeking Symmetries between Self-Assembly of Heteronucleants and Crystals
- **Fiora Artusio**, Giacomo Ceccone, Roberto Pisano
- **5:10** Paper 600e: Olanzapine Crystal Symmetry Originates in Preformed Centrosymmetric Solute Dimers

 Peter Vekilov
- **5:35** Paper **600f**: Development of a Hybrid Quality-By-Control Framework for Optimal Crystallization Process Design
- **Ayse Eren**, Botond Szilagyi, Justin L. Quon, Charles D. Papageorgiou, Zoltan K. Nagy
- (601) Particulate and Multiphase Flows: Foams and Bubbles Wednesday, Nov 13, 3:30 PM

Hyatt Regency Orlando, Orlando Ballroom L Ya-Wen Chang, Co-Chair

Charles E. Sing, Co-Chair Javen Weston, Co-Chair Christopher L. Wirth, Co-Chair

Sponsored by: Fluid Mechanics

- **3:30 Paper 601a:** Coating and Crumpling of Armored Gas Filled Capsules
- Charles Sharkey, Zixian Cui, Shelley L. Anna
- **3:45** Paper 601b: Optimal Investigation on Heat Transfer and Hydrodynamics in a Gas-Solid Fluidized Bed with Vertical Immersed Internals
- **Jiantao Li**, Lu Liu, Xiuying Yao, Chunxi Lu
- **4:00 Paper 601c:** Effect of Inlet Geometry on Gas-Liquid Two-Phase Flow in a Horizontal Pipeline
- Carla Nayara Michels dos Santos, Sarah Laysa Becker, Vinícius Basso Godoy, Celso Murilo dos Santos, Christine Fredel Boos, **Marcela Kotsuka da Silva**, Henry França Meier
- **4:15** Paper 601d: Fundamental Experimental Analysis of Single Bubble Breakup in Stirred Tanks By 3D-Particle Tracking
- Frederic Krakau, Matthias Kraume
- **4:30 Paper 601e:** Characterization of the Bubble Swarm Trajectory in a Jet Bubbling Reactor
- **Yun Shuai**, Xiaoyun Guo, Haotong Wang, Zhengliang Huang, Yao Yang, Jingyuan Sun, Jingdai Wang, Yongrong Yang
- **4:45** Paper 601f: Experimental Study of Dynamics of Clusters for Geldart a and B Particles in a Circulating Fluidized Bed Riser Using Movable ECT
- Naval Koralkar
- **5:00** Paper **601g**: Quantifying Effects of Coarse-Grain Model Parameter in CFD-DEM Simulations of Fluidized and Spouted Beds and Comparison Against Eulerian Multiphase Simulation Results
- **Thomas Eppinger**, Chandra Tourani, Ravindra Aglave
- **5:15 Paper 601h:** Microfluidic Measurement of the Interfacial Tension of the Water-Diluted Bitumen Interface
- Sachin Goel, Samson Ng, Edgar Acosta, **Arun Ramchandran**, Mohammad Uddin, Niyati Joshi
- **5:30 Paper 601i:** CFD Simulation of Solid-Liquid Separation in Lab-Scale Centrifuge and Comparison to Experimental Data
- **Tojonirina Randriamanantena**, Lea Rouquette, Laure Hejl, Denis Ode
- **5:45 Paper 601j:** Evaporation Driven Oscillatory Marangoni Flow in Thin Films of a Binary Mixture
- **Xingyi Shi**, Gerald G. Fuller, Eric Shaqfeh
- (602) Polymer Processing and Rheology

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 5 Blair Kathryn Brettmann, Chair Keith Forward, Co-Chair

Sponsored by: Polymers

- **3:30** Paper **602a**: 3D Printing of Polymer-Bonded Magnets from Highly Concentrated Suspensions
- Alan Shen, Xiaoguang Peng, Callum Bailey, Sameh Dardona, **Anson Ma**
- **4:00** Paper 602b: Multiscale Rheological Investigation of Highly Filled Multi-Layer Filament for Fused Deposition Modeling (FDM)
- Rebecca Ruckdashel, Shihang Wang, **Jay Park**, Javier Vera-Sorroche
- **4:15** Paper 602c: Residence Time Distribution in a Chilled Polymer Extruder: Solid-State Shear Pulverization (SSSP)
- Philip R. Onffroy, Evan V. Miu, William J. Confer, Caleb M. Darkes-Burkey, Katsuyuki Wakabayashi
- **4:30 Paper 602d:** Reversibly Cross-Linked Nonwoven Fibers: Sustainability Meets Melt Blowing
- **Kailong Jin**, Aditya Banerji, David Kitto, Jun Xu, Sung-soo Kim, Frank S. Bates, Christopher J. Ellison
- **4:45** Paper **602e**: Structure-Property Relationships Via Recovery Rheology in Polymeric Materials
- **Johnny Ching-Wei Lee**, Katie Weigandt, Elizabeth G. Kelley, Simon Rogers
- **5:00** Paper 602f: Macromolecular Dynamics and Extensional Rheology of Aqueous Solutions of Flexible and Semi-Flexible Polymers
- Jelena Dinic, Vivek Sharma
- **5:15 Paper 602g:** The Sensitivity of Extensional Rheology to Long Chain Branching in Commercial Polyethylene Samples
- Samantha L. Morelly, **Nicolas J. Alvarez**
- **5:30 Paper 602h:** Elucidating the Molecular Rheology of Entangled Polymeric Fluids Via Direct Comparison of NEMD Simulations and Model Predictions
- Mohammad Hadi Nafar Sefiddashti, Brian J Edwards, **Bamin Khomami**
- (603) Polymers in Additive Manufacturing

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 27 Mingjiang Zhong, Chair Michael J. Bortner, Co-Chair

Sponsored by: 3D Printing

- **3:30 Paper 603a:** Flow-Induced Crystallization in Materials Extrusion Additive Manufacturing
- Anthony P. Kotula
- **4:00** Paper 603b: Computational Fluid Dynamics Simulation of the Fused Deposition Modeling Process: Effect of Temperature-Dependent Viscosity on the Shape of Extruded Strand
- **Behrouz Behdani**, Leah Mason, Ming Leu, Joontaek Park

- 4:20 Paper 603c: Effect of
 Polypropylene Melt Flow Index on
 the Material Extrusion Based Additive
 Manufacturing of Polypropylene/
 Hydrogenated Resin Blends
 Arit Das, Emma M. Dartevelle,
 Eugene G. Joseph, Michael J. Bortner
- **4:40** Paper 603d: Engineering Filament Design for Enhanced Printability and Mechanical Properties of Additively Manufactured Plastic Parts *Bryan D. Vogt*
- **5:00 Paper 603e:** 3D Printing of Interdigitated Dielectric Elastomer Actuators
- **Alex Chortos**, Ehsan Hajiesmaili, David R. Clarke, Jennifer A. Lewis
- **5:20 Paper 603f:** Direct Print Additive Manufacturing of Optical Fiber Interconnects for Board Level Computing Devices
- **Roger B. Tipton**, Dianhao Hou, Thomas M. Weller, Venkat R. Bhethanabotla
- **5:40** Paper **603**g: Curethrough Correction in Continuous Stereolithographic 3D Printing

 Zachary D. Pritchard, Martin de Beer, Timothy F. Scott, Mark A. Burns

(604) Polymer Thin Films, Nanoconfinement, and Interfaces II Wednesday, Nov 13, 3:30 PM

Hyatt Regency Orlando, Celebration 15 Laura Bradley, Chair Christian W. Pester, Co-Chair

Sponsored by: Polymers

- **3:30** Paper 604a: Giant Hyaluronan Polymer Brushes Display Polyelectrolyte Brush Polymer Physics Behavior
 Jessica Faubel, Riddhi Patel,
 Jennifer Curtis, Blair Kathryn
 Brettmann
- **3:45 Paper 604b:** Manipulation of Surface Chemistry Via Polymer Chain-End Segregation in Topologically Constrained Materials
- **Caroline Szczepanski**, John M. Torkelson
- **4:00** Paper 604c: Segregation of Bottlebrush Copolymer Additives to Thin Film Interfaces
- **Hao Mei**, Travis Law, Jiabei Li, Gila Stein, Rafael Verduzco
- **4:15** Paper **604d**: Well-Defined Polymer Adhesives Synthesis: Pendant Functionalities and Crosslinking Effect on Properties
- Hoyong Chung
- **4:30** Paper 604e: Molecular Layer Deposition: Mechanisms of Vapor-Phase Organic Ultrathin Film Synthesis
- **David S. Bergsman**, Richard G. Closser, Christopher J. Tassone, Bruce M. Clemens, Dennis Nordlund, Stacey F. Rent

- **4:45** Paper **604f**: Bottom-up Fabrication of Flexible and Porous Omniphobic Interfaces Via Sequential Initiated Chemical Vapor Deposition *Mahdi Mohammadi Ghaleni*, Shayan Kryigni Mong Rayarian Signer
- **Mahdi Mohammadi Ghaleni**, Shayan Kaviani, Mona Bavarian, Siamak Nejati
- **5:00 Paper 604g:** Robust Polymer Coatings for Controlling CaCO₃ Heterogeneous Nucleation in Thermal Desalination
- **Junjie Zhao**, Minghui Wang, Karen K. Gleason
- **5:15** Paper 604h: Magnetic- and Light-Driven Wettability Switching of Fluorinated Ionic Liquid Infused Slippery Surfaces
- **Qingqing Rao**, Qinghua Zhang, Xiaoli Zhan, Fengqiu Chen
- **5:30** Paper **604i**: Exploring Zone Specific Proton Transport of Ionomers Under Confinement Via Confocal Laser Scanning Microscopy
- **Seefat Farzin**, Shudipto Konika Dishari
- **5:45** Paper 604j: Humidity-Responsive Patternable Multilayer Nanofilms with Fast Tunable Colors
- Ziye Dong, Wei Li

(605) Predictive Scale-up/ Scale-down for Production of Pharmaceuticals and Biopharmaceuticals II

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 7 Kushal Sinha, Chair Jerry S. Salan, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **3:30** Paper 605a: Computation Fluid Dynamics (CFD) Guided Design of Single Use Bioreactors (SUBs) at Bench Scale *William Tran*
- **3:50 Paper 605b:** CFD Analysis of Micro and Macro Mixing for Robust Scale-up of Addition Rate and Impellor Speed
- **Veera Pratap R. Kasina**, Samir T. Hasan**, Birendra K. David**
- **4:10** Paper **605c**: Physics-Based Modeling of Free Surface Dynamics Using Graphics Processing Units (GPUs) *Brian DeVincentis*, *John A. Thomas, Kevin Smith*
- **4:30** Paper 605d: Challenges in Transfer of a Shear Sensitive Lubricated Formulation from a Dosator-Type to a Dosing Disk-Type Capsule Filling Machine *Mehrdad Kheiripour, Richard Moore, Mello Hebert, Bonnie Le, James*
- **4:50 Paper 605e:** A Quality By Design Approach to Address the Challenges of Direct Compression Scale-up and Technology Transfer between Rotary Tablet Presses

Henshilwood

— **Raghu V. G. Peddapatla**, Gerard Sheridan, Conor Slevin, Shrikant Swaminathan, Ivan Browning, Clare O' Reilly, David Egan, Stephen Sheehan, Abina Crean

- **5:10 Paper 605f:** Scale-up of Roller Compaction Processes Using a Geometric Scaling Model
- Trinkle David
- **5:30** Paper 605g: Local Residence Time Distributions for Hot Melt Extrusion: Making a Black Box Concept Mechanistic
- Hannes Bauer, **Josip Matić**, Johannes G. Khinast
- **5:45** Paper **605h**: Simulation Aided Pharmaceutical HME Scale-up *Josip Matić*, Abdelhamid Mostafa, Carolina Alva, Johannes G. Khinast

(606) Process Intensification through Process Systems Engineering

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Bayhill 24 Fernando V. Lima, Chair Maria Papthanasiou, Co-Chair

Sponsored by: Systems and Process Design

- **3:30 Paper 606a:** Multiscale Modeling of Liquid-Liquid Phase Transfer Catalysis for the Simultaneous Extraction and Conversion of Hydrogen Sulfide to Value-Added Products
- Abhimanyu Pudi, Vahid Shadravan, **Adam Karcz**, Seyed Soheil Mansouri, Martin Andersson
- **3:49** Paper 606b: Optimization of Syngas to Olefin (STO) Reactors

 Can Ekici, Lorenz T. Biegler, Joseph DeWilde, Dylan Kipp, Paul Witt
- **4:08** Paper 606c: Sustainable Process Intensification Using Building Blocks *Salih E. Demirel, Jianping Li, M. M. Faruque Hasan*
- **4:27 Paper 606d:** Batch to Continuous (B₂C) Reactor Intensification through a First-Principles-Based Optimization Framework
- **Joseph Costandy**, Thomas F. Edgar, Michael Baldea
- **4:46** Paper 606e: Development of Process Operability Algorithms for Modularization and Intensification of Energy Systems
- Vitor Gazzaneo, Fernando V. Lima
- **5:05** Paper 606f: A Modular Approach to Process Integration and Intensification
- **Yuhe Tian**, losif S. Pappas, Styliani Avraamidou, Efstratios N. Pistikopoulos
- **5:24** Break
- **5:43** Paper 606h: Mathematical Optimization and Process Intensification of Diafiltration Membrane Systems
- **Elvis Eugene**, William A. Phillip, Alexander W. Dowling

(607) Protein Engineering Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 1

Hyatt Regency Orlando, Celebrati Kevin J. Cash, Chair Jerome M. Fox, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30** Paper 607a: Designing with Nanoscale Building Blocks: Engineering Self-Assembling Protein Superstructures for Applications in Vaccines, Drug Delivery and Biochemical Production Danielle Tullman-Ercek
- **4:10** Paper 607b: Developing Formate Dehydrogenase into a Modular Cofactor Regeneration and Sequestration Tool

 Nadim Massad, Scott Banta
- **4:28 Paper 607c:** Calamri: Calcium Activated MRI Reporters for Imaging Neuroactivity
- Harun Ozbakir, Arnab Mukherjee
- **4:46 Paper 607d:** Rosetta-Inspired Design of Conformationally Constrained Cylic Anti-Amyloid Peptides
- **Chandler Est**, Parth Mangrolia, Regina M. Murphy
- **5:04** Paper **607e**: Understanding the Structural Basis of Protein Activation By Tuning the Pka of an Embedded Charge *Chung-ta Han*, *Khrysta Pruett, Jichao Song, Song-I Han*
- **5:22 Paper 607f:** A Coarse-Grained Model to Elucidate the Regulation of Protein Phase Behavior By Post Translational Modifications
- **Theodora Myrto Perdikari**, Gregory L. Dignon, Jeetain Mittal, Nicholas Fawzi
- **5:40** Paper **607g**: Synthesis and Characterization of a Novel Protac Containing a β-Hairpin Sequence Motif to Selectively Knockdown Tau Protein Hannah C. Hymel, Jeffery C. Anderson, Jacob H. Pettigrew, Ted J. Gauthier, Adam T. Melvin

(608) Protein Science and Engineering: High Throughput Screening and Characterization Wednesday, Nov 13, 3:30 PM

Wednesday, NoV 13, 3:30 PM
Hyatt Regency Orlando, Celebration 3
Aditya M. Kunjapur, Co-Chair
Jason T. Boock, Co-Chair
Daniel Woldring, Co-Chair

Sponsored by: Bioengineering

- **3:30 Paper 608a:** Novel High-Throughput Technology for Antibody Discovery Synthesizing the Virion Display and Yeast Display Platforms *Jamie B. Spangler*
- **3:48** Paper 608b: Chemically Diverse Peptide Libraries Yield Potent Inhibitors of the p₅₃-MDM₂ Interaction
 Tejas Navaratna, *Greg Thurber*
- **4:06** Paper 608c: Quantitative Analysis of Protein-Protein Interactions Using a Yeast-Yeast Two Hybrid Model

 Knithyn Recom Abjacil Blain
- **Kaitlyn Bacon**, Abigail Blain, Matthew Burroughs, Nikki McArthur, Stefano Menegatti, Balaji Rao
- **4:24** Paper 608d: Strategies for Expanding Genetically Encoded Chemical Diversity in Yeast

 Jessica T. Stieglitz, James A. Van Deventer

- **4:42 Paper 608e:** Collateral Fitness Effects of Mutations
- Jacob D. Mehlhoff, Frank W. Stearns, Dahlia Rohm, Buheng Wang, Erh-Yeh Tsou, Meng-Hsuan Hsiao, Nisita Dutta, Alan F. Rubin, Courtney E. Gonzalez, Marc Ostermeier
- 5:00 Paper 608f: Machine-Learning Guided Mutagenesis for Directed Evolution of Recombinant Proteins — Yutaka Saito, Misaki Oikawa, Hikaru Nakazawa, Tomoshi Kameda, Koji Tsuda, Mitsuo Umetsu
- **5:18** Paper 608g: High-Throughput Screens and Selections for Enzyme Function in Non-Model Bacteria

 Joshua K. Michener
- (609) Self-Assembled Biomaterials Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Discovery 44

Anju Gupta, Chair Alexander E. Marras, Co-Chair

Sponsored by: Bionanotechnology

- **3:30** Paper 609a: Self-Assembled ssDNA Nanotubes for Targeting Cancer (Invited Speaker)

 Efie Kokkoli
- **4:00** Paper **609b**: Self-Assembly of Hydrophobically-Patterned Charged Polypeptides for Drug Delivery

 Sara Tabandeh, *Lorraine Leon*
- **4:20 Paper 609c:** Dynamic, Reversible Control of Biomaterial Properties Using DNA
- Nicholas Stephanopoulos
- **4:40** Paper 609d: Peptoid Microsphere Coatings: The Effects of Helicity, Temperature, pH, and Ionic Strength Jesse Roberts, German Perez, Bryce Colford, Shannon L. Servoss
- **5:00** Paper **609e**: Cationic, Anionic, and Amphoteric Dual pH/Temperature-Responsive Degradable Microgels Via Self-Assembly of Functionalized Oligomeric Precursor Polymers
- **Eva Mueller**, Madeline Simpson, Sebastian Himbert, Michael Majcher, Gero Padberg, Ana Arezina, Ridhdhi Dave, Todd R. Hoare
- **5:20** Paper 609f: Calcium-Phosphate Supraparticle Assembly Is Influenced By Both Intermolecular Forces and Fluid Dynamics
- **Adam A. Caparco**, Andreas S. Bommarius, Julie A. Champion
- **5:40** Paper **609g**: Interaction of Amphiphilic Coumarin with DPPC/DPPS Using DSC and MD Simulations: Effects of Concentration and Chain Length *Anju Gupta*, *Poornima Kalyanram*, *Shikha Nangia*, *Istvan Stadler*
- (610) Solid-Fluid Separations in Oil & Gas Production and Refining Processes

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Coral Spring I/II Isaac K. Gamwo, Chair

Sponsored by: Fluid-Particle Separations

- **3:30** Paper 610a: Advances in Gas-to-Liquid Solid-Liquid Separation Systems — *Seyi A. Odueyungbo*
- Seyi A. Odueyungbo
- **3:55 Paper 610b:** Separation Characteristics in a Novel Gas-Liquid Vortex Separator
- **Wen Zhou**, Kangsong Wang, Chenalin E. Chunxi Lu
- **4:20 Paper 610c:** Magnetophoretic Capture of 5 Nm Sized Superparamagnetic Iron Oxide Nanoparticles Under Different Gradient Field Conditions
- **Jenifer Gómez-Pastora**, Xian Wu, Mitchell Weigand, James Kim, Maciej Zborowski, Lee Moore, Jeffrey J. Chalmers
- **4:45 Paper 610d:** Bubbly Flow in Degassing Cyclones and Potential Applications
- **Xiao Xu**, Qiang Yang, Hualin Wang, Honglai Liu

(611) Sustainable Food Production Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Celebration 9 David E. Block, Chair

Sponsored by: Food Innovation and Engineering

- **3:30** Paper 611a: Evaluation of Ultrasound By Direct Contact on Convective Drying of Banana (*Musa paradisiaca*) Slices Using Principal Component Analysis and Response Surface Methodology
- **Erika K. Méndez**, Carlos E. Orrego, Enrique J. De la Hoz
- **3:55 Paper 611b:** Energy Usage in Food Manufacture
- Alia Ladha-Sabur, Peter J. Fryer, Serafim Bakalis**, Estefania Lopez-Quiroga**
- **4:20** Paper 611c: Sustainability of Nano-Packaging Use for Food Shelf Life Extension: Life Cycle Assessment Perspective
- Bruce Y. Zhang, Yifan Tong, Soumya Singh, Hua Cai, **Jen-Yi Huang**
- **4:45 Paper 611d:** Placeholder Talk Paul Bowen
- Paul Bowen
- **5:10 Paper 611e:** Placeholder Talk
- 5:35 Paper 611f: Placeholder Talk

(612) Systems and Quantitative Biology: Modeling Biological Processes

Wednesday, Nov 13, 3:30 PM
Hyatt Regency Orlando, Celebration 4
Nanette R. Boyle, Co-Chair
Clayton Jeffryes, Co-Chair
Rajib Saha, Co-Chair
Laura Jarboe, Co-Chair

Sponsored by: Bioengineering

- **3:30 Paper 612a:** A Mathematical Model to Reproduce Biphasic DNA Amplification Output
- Burcu Ozay, Danielle Ciesielski, Tomas Gedeon, **Stephanie McCalla**
- **3:48 Paper 612b:** The Low-Pass Filtering Effect of Degradation-Driven Protein Turnover
- Bahareh Mahrou, Azady Pirhanov, Yong-Jun Shin, **Yongku Cho**
- **4:06** Paper 612c: Evolution of Modular Networks through Optimal Sparse Control
- Pedro Constantino, Wentao Tang, **Prodromos Daoutidis**
- **4:24** Paper 612d: From 13c Labeling Data to a Core Metabolism Kinetic Model: A Kinetic Model Parameterization Pipeline
- Charles Foster, Saratram Gopalakrishnan, Shyam Srinivasan, Satyakam Dash, Maciek R. Antoniewicz, Costas D. Maranas
- **4:42** Paper **612e**: Defining the Architecture of Complex Traits to Enable Genome Design
- **Christopher M. Jakobson**, José Aguilar-Rodríguez, Thomas Lozanoski, Zachary Harvey, Richard She, Daniel F. Jarosz
- **5:00 Paper 612f:** A Network Reduction Tool for Compressing and Visualizing Genome-Scale Metabolic Models
- **Daniel Lugar**, Ganesh Sriram
- **5:18 Paper 612g:** Invited Talk for Modeling Biological Processes *Nanette R. Boyle*

(613) Thermochemical Conversion of Biomass

Wednesday, Nov 13, 3:30 PM Hyatt Regency Orlando, Discovery 47 Chang Geun Yoo, Chair Michael T. Timko, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

- **3:30 Paper 613a:** Pyrolysis and Steam Gasification Characteristics of Mangroves Under Rapid Heating Conditions
- **Yuya Sakurai**, Yuji Sakai, Jun Kobayashi
- **3:50 Paper 613b:** Super Activated Hydrochar for Hydrogen Storage
- **Nepu Saha**, M.Toufiq Reza
- **4:10 Paper 613c:** Investigations of Properties of Carbon Quantum Dots Obtained from Hydrothermally Carbonized (HTC) Process Liquids
- Md. Rifat Hasan, M.Toufiq Reza
- **4:30** Paper 613d: Wet Biomass Waste Valorization through Hydrothermal Liquefaction and Integrated Post-Treatment Measures
- **Kui Wang**, Qiulin Ma, Hanifrahmawan Sudibyo, Jillian L. Goldfarb, Jefferson W. Tester

- **4:50 Paper 613e:** Scale up and Product Validation of Biomass Derived Sugar to Acrylonitrile Process
- **Jadid E. Samad**, Swanand Tupsakhare, Zora Govedarica, Amit Goyal, Jeremy Moskowitz, Billy Harmon
- **5:10** Paper 613f: Fate of Inorganics during Hydrothermal Carbonization of High Ash Fraction of Air Classified Biomass
- Nepu Saha, Kyle McGaughy, Omid Norouzi Safsari, Tyler L. Westover, **M.Toufiq Reza**
- **5:30 Paper 613g:** High-Quality Biocrude Production from Reactive Catalytic Fast Pyrolysis
- Joseph Weiner

(614) Ammonia as an Energy Carrier Wednesday, Nov 13, 4:00 PM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

- **4:00 Paper 614a:** Ammonia as an Energy Carrier Update from the Netherlands
- Johannes Pieter Vrijenhoef
- **4:23** Paper 614b: Case Study of Ammonia Production in the Island States Using Ocean Thermal Energy *C. B. Panchal*
- **4:46 Paper 614c:** Ammonia As Hydrogen Carrier to Unlock the Full Potential of Green Renewables
- **Camel Makhloufi**, Pierre Olivier, Nouaamane Kezibri, Alexi Liedes
- **5:09 Paper 614d:** Green Ammonia Production Integrated into US Wholesale Power Markets
- Shaun Mann

(615) William R. Schowalter Lecture Wednesday, Nov 13, 6:00 PM Hyatt Regency Orlando, Plaza International Ballroom H Pablo G. Debenedetti, Chair

Sponsored by: Liaison Functions

6:00 Paper **615a**: Flowing Complex Fluids, from Blood to the Buffer Layer — *Michael D. Graham*

(616) Ammonia Energy Association: Platinum Reception

Wednesday, Nov 13, 6:00 PM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

- **6:00** Paper 616a: Decarbonized Ammonia for Food and Energy *Rob Stevens*
- 6:23 Reception

(617) Ammonia Synthesis: Next Generation Technology II

Thursday, Nov 14, 8:00 AMHyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

- 8:00 Introductory Remarks
- **8:03** Paper 617a: Comparative Technoeconomic Analysis of Conventional and Absorbent-Enhanced Ammonia Synthesis
- **Matthew J. Palys**, Alon McCormick, E. L. Cussler, Prodromos Daoutidis
- **8:26 Paper 617b:** Yittria-Stabilized Zirconia (YSZ) Supports for Low Temperature Ammonia Synthesis
- **Zhenyu Zhang**, Sarah Livingston, Lucy Fitzgerald, Thomas F. Fuerst, Simona Liguori, J. Douglas Way, Colin A. Wolden
- **8:49** Paper 617c: An Integrated Evaluation Method with Application to a New Ammonia Synthesis Process Design
- Jia Li
- **9:12** Paper **617d:** Effect of Preparation Condition on Ammonia Synthesis over Ru/CeO.
- **Tetsuya Nanba**, Keisuke Kobayashi, Yuuki Nagata, Javaid Rahat, Hideyuki Matsumoto
- **9:35** Paper 617e: Ammonia Absorbents with High Stability and High Capacity for Fast Cycling
- Matthew Kale, Joshua I. Militti, Sayandeep Biswas, Alon McCormick, Paul Dauenhauer, E. L. Cussler

(618) Accelerated Discovery and Development of Inorganic Materials

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Celebration 16
Sankar Nair, Chair
Dongxia Liu, Co-Chair
Satish K. Nune, Co-Chair

Sponsored by: Inorganic Materials

- **8:00 Paper 618a:** Metal Organic Framework Materials for Sound Attenuation Applications
- Satish K. Nune, Quin Miller, Herbert T. Schaef, Kayte Denslow, Paul Martin, B. Peter McGrail
- **8:18** Paper 618b: MOFs and COFs for Alternative Operating Conditions for Hydrogen Storage Explored by Machine Learning
- Grace Anderson, Benjamin Schweitzer, Ryther Anderson, **Diego Gomez Gualdron**
- **8:36** Paper 618c: Role of Ce in Manipulating Tb Luminescence in Y₂Zr₂O₂ Nanoparticles Yuming Wang, James A. Dorman
- 8:54 Paper 618d: Synthesis
- and Complex Electrochemistry of Manganese Dioxide in Alkaline Batteries — *Gautam G. Yaday*
- **9:12 Paper 618e:** Pseudocapacitive Storage in Nanolayered Ti₂NTx mxene Using Mq-Ion Electrolyte
- **Abdoulaye Djire**, Andre Bos, Jun Liu, Hanyu Zhang, Elisa Miller, Nathan Negle

- 9:30 Paper 618f: Oxidation and Stabilization of 2D Mxene Nanosheets Xiaofei Zhao, Touseef Habib, Evan Prehn, Aniruddh Vashisth, Smit Shah, Jodie L. Lutkenhaus, Miladin Radovic, Micah J. Green
- **9:48** Paper **618g:** Multilevel Structured Electrospun Ceramic Nanofibers and Their Potential Applications in the Energy Sector
- Oren Elishav, Gennady E. Shter, Gideon S. Grader

(619) Adsorbent Materials Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Manatee Spring I

Joshua Thompson, Chair Dipendu Saha, Co-Chair

Sponsored by: Adsorption and Ion Exchange

- 8:00 Paper 619a: Novel Al-Rich Chabazite Compositions Enable Ar PSA — Anthony Vallace, Grant Kester, William Casteel Jr., Garret Lau, Roger D. Whitley, Charles Coe
- **8:20 Paper 619b:** A Porous Organic Cage's Structural Evolution through Time
- **Jolie Lucero**, Sameh Elsaidi, Ryther Anderson, Ting Wu, Diego Gomez Gualdron, Praveen K. Thallapally, Moises A. Carreon
- **8:40** Paper 619c: Removal of H₂S and CO₂ from Raw Natural Gas Using Wood Fly Ash from Alberta Kraft Pulp Mills

 Jing Jing CAI, Paolo Mussone
- **9:00 Paper 619d:** A Technical Overview about the Use of Ultra-Microporous Fluorinated MOF for Separations and Sensing Applications
- Youssef Belmabkhout
- **9:20 Paper 619e:** Study of Lanthanum Carbonate Nanowire for Adsorption of Phosphorus: Material Synthesis and Optimization and Demonstration of Performance
- **Kok Yuen Koh**, Sui Zhang, J. Paul Chen
- **9:40** Paper 619f: Development of Oxygen-Selective Sorbents for Low- and High-Temperature Air Separation
- **Qinghe Zheng**, Marty Lail, Shaojun Zhou
- **10:00 Paper 619g:** Fabrication of Metal-Organic Framwork Nanosheets@ Cellulose Composites As Adsorbents for Organic Solvent Recovery
- Xueyi Zhang, Jie Zha

(620) Advanced Treatment for Water: Reuse and Recycling

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Rainbow Spring I/II

Sage R. Hiibel, Chair M. Toufiq Reza, Co-Chair

Sponsored by: Water

- **8:00** Paper **620a**: Reclaiming Phosphorus from Secondary Treated Municipal Wastewater with Engineered Biochar
- **Yulin Zheng**, Bing Wang, Anne Wester, Jianjun Chen, Feng He, Hao Chen, Bin Gao
- **8:17** Paper 620b: Nutrient Recovery from Municipal Wastewater Using a Methanotroph-Microalgae Co-Culture Nathan Roberts, Q. Peter He, Jin
- **8:34 Paper 620d:** Removal of Organics, Metals, Microbes, and Algae Using Electro-Magnetic Fields
- Phil Carlberg, Kurt Swogger
- **8:51 Paper 620e:** Coupled Membrane Distillation-Crystallization for Water and Salt Recovery from High-Strength Brine
- Sage R. Hiibel, Evangelos Balis
- 9:08 Break
- **9:25** Paper 620g: An Asymmetric Iron-Based Redox-Active System for Electrochemical Ion Separation in Aqueous Media
- **Kai-Jher Tan**, Xiao Su, T. Alan Hatton

(621) Advances in Optimization: Global, Surrogate & Mixed-Integer Models II

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 24 Kody Powell, Chair Tony Wu, Co-Chair

Sponsored by: Computers in Operations and Information Processing

- **8:00 Paper 621a:** Decomposition in Derivative-Free Optimization
- **Kaiwen Ma**, Nikolaos V. Sahinidis, Satyajith Amaran, Sreekanth Rajagopalan, Scott J. Bury
- **8:18 Paper 621b:** Mixed-Integer Multi-Objective Optimization through Multiparametric Programming
- **Styliani Avraamidou**, Justin Katz, Baris Burnak, Burcu Beykal, Iosif S. Pappas, Metin Turkay, Efstratios N. Pistikopoulos
- **8:36 Paper 621c:** Global Optimization of Nonconvex Quadratic Programs and Mixed-Integer Quadratic Programs
- **Carlos Nohra**, Arvind Raghunathan, Nick Sahinidis
- **8:54 Paper 621d:** Surrogate-Based Optimization for Mixed-Integer Nonlinear Problems
- **Sun Hye Kim**, Fani Boukouvala
- **9:12 Paper 621e:** An Algorithm for the Exact Solution of Multiparametric Quadratically Constrained Quadratic Programming Problems
- **losif S. Pappas**, Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos
- 9:30 Paper 621f: Strengthened Socp Relaxation and Efficient Hybrid Bounds Tightening Scheme for the Global Solution of AC Optimal Power Flow Problems
- **Yuanxun Shao**, Joseph Scott

- **9:48** Paper **621g**: Multistage Adaptive Mixed Integer Optimization Using Improved Piecewise Decision Rule Farough Motamed Nasab, **Zukui Li**
- **10:06 Paper 621h:** Computing Subgradients of Bivariate Functions for Nonsmooth Optimization
- Kamil A. Khan

(622) Alternative Fuels including Biofuels, Hydrogen, and Syngas Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 29/30 Hemant P. Pendse, Chair

Sponsored by: Transport and Energy Processes

- **8:00 Paper 622a:** Carbon Dioxide Removal from Biogas Using Amine Based Silica Sorbents
- Umadevi Gopalakrishnan, J. N. Kuhn, Babu Joseph
- 8:25 Paper 622b: Promoted
 Effect of D-Mannitol on Thermal
 Dehydrogenation of Ammonia Borane
 Geo-Jong Kim, Alisha Boone, Hyun-Tae Hwang
- **8:50 Paper 622c:** Techno-Economic Feasibility of Thermocatalytic Conversion of CO₂ into Renewable Natural Gas (RNG)
- Sogol Mottaghi-Tabar, **David Simakov**
- **9:15** Paper 622d: High-Pressure Hydrogen Production from Bio-Ethanol Feedstock with Fixed-Bed Chemical Looping
- Robert Zacharias, Sebastian Bock,
 Karin Malli, Viktor Hacker
- **9:40** Paper 622e: Biohydrogen Production from Gamma Irradiation Disintegrated Sewage Sludge: Effect of Ferrous Ions
- Yanan Yin

(623) Anisotropic Particles: Synthesis, Characterization, Modeling, Assembly, and Applications

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Orlando Ballroom N

Bhuvnesh Bharti, Chair Sepideh Razavi, Co-Chair

Sponsored by: Interfacial Phenomena

- **8:00 Paper 623a:** Synergies between Heterogeneous Nanoparticles and Surfactants to Stabilize Emulsions
- **Tuan V. Vu**, Dimitrios V. Papavassiliou

Chen, Tianyu Yan

- **8:15 Paper 623b:** Dynamics and Rheology of Suspensions of Particles with Arbitrary Shapes
- Mingyang Tan, Joshua A. Adeniran, **Travis W. Walker**
- **8:30** Paper 623c: Growth Mechanism of Five-Fold Twinned Ag Nanowires from Multi-Scale Theory and Simulations

 Kristen Fichthorn, Xin Qi, Zihao

- **8:45** Paper **623d**: A Novel Nano-Lithographic Pathway for Fabricating Anisotropic Nanoparticles of Different Shape and Composition
- **Tanweepriya Das**, Md. Hemayet Uddin, Raymond R. Dagastine
- **9:00** Paper **623e**: Quantifying Anisotropic Properties Emerging from Uniformly Coated Gold Nanoparticles *Alex K. Chew, Reid C. Van Lehn*
- **9:15** Paper 623f: Direct Observation of the Dynamics of Mono- and Multi-Layer 2D Materials at Fluid-Fluid Interfaces *David M. Goggin*, *Hanyu Zhang*, *Elisa Miller*, *Joseph R. Samaniuk*
- **9:30** Paper 623g: Influence of Cap Weight on the Motion of a Janus Particle Very Near a Wall
- **Aidin Rashidi**, Sepideh Razavi, Christopher L. Wirth
- **9:45** Paper **623h**: Brownian Dynamic Simulation of the Motion of a Janus Particle Near a Boundary and Under Shear Flow
- **Zohreh Jalilvand**, Ilona Kretzschmar, Joel Koplik
- **10:00 Paper 623i:** Magnetic Field Driven Assembly of Multicomponent Low-Symmetry Supraparticles

 Ahmed Al Harraq, Jin Gyun Lee,

 Bhuvnesh Bharti

(624) Biological Conversions and Processes for Renewable Feedstocks

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Regency Ballroom T Hasan K. Atiyeh, Chair Shishir Chundawat, Co-Chair Rebecca Ong, Co-Chair

Sponsored by: Sustainable Biorefineries

- **8:00 Paper 624a:** Roller Bottle Method to Generate High-Solids, Fermentable Enzymatic Hydrolysates and Rapidly Screen Plant Materials
- Emily Burke, Meenaa Chandrasekar, Leela Joshi**, Rebecca Ong**
- **8:20** Paper 624b: Effect of Carbonyl Inhibitors on the Intracellular Metabolism in Microbial Fermentation *Yu Zhang, Maobing Tu*
- **8:40** Paper 624c: Supplementation of Growth Medium with Biochar Enhances Production of Acetone-Butanol-Ethanol from Switchgrass By *Clostridium Beijerinckii*
- Xiao Sun, **Hasan K. Atiyeh**, Yinka Adesanya, Hailin Zhang, Christopher Okonkwo, Thaddeus Ezeji
- **9:00** Paper **624d**: Mass Balance Based Semi-Quantification of Adipic Acid Producing Enzyme Cascade
- **Nicholas S. Kruyer**, Andreas S. Bommarius, Pamela Peralta-Yahya
- **9:20** Paper **624e**: Production of Optically Pure L-Lactic Acid from Paper Sludge By Bacillus Coagulans
 Jing Li, Zhihua Jiang

- **9:40** Paper **624f**: Design and Modification of the Upstream Process in a Biorefinery By Modeling and Combined Uncertainty and Sensitivity Analysis
- **Nikolaus I. Vollmer**, Celina K. Yamakawa, Krist V. Gernaey, Solange I. Mussatto, Gürkan Sin

(625) Biomaterial Scaffolds for Tissue Engineering

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Celebration 10
R. Michael Gower, Chair
Jungwoo Lee, Co-Chair
Gulden Camci-Unal, Co-Chair
Samira M. Azarin, Co-Chair

Sponsored by: Biomaterials

- **8:00 Paper 625a:** Cancer Self-Organization Using Collagen Poly (ethylene qlycol) Hydrogel Matrix Modulation
- **Kathryn M. Sullivan**, John D. Ito, William Ballance, Mikhail Kandel, Byoungsoo Kim, Gabriel Popescu, Hyunjoon Konq
- **8:18** Paper **625b**: Resveratrol Loaded PLG Scaffolds Prevent Accumulation of Epididymal Adipose Tissue after High Fat Diet Challenge
- **Kendall Murphy**, Michael Hendley, Christopher Isely, Michael Gower
- **8:36** Paper **625**c: Differential Effects of Heparin and Hyaluronic Acid on Neural Patterning of Human Induced Pluripotent Stem Cells
- Julie Bejoy, Yan Li
- 8:54 Paper 625d: Collagen Type I and II Blend Hydrogels with Mesenchymal Stem Cells As Scaffolds for Articular Cartilage Defect Repair
- Claire Kilmer, Abigail Durkes, Gert Breur, Alyssa Panitch, Julie C. Liu, **Carly Battistoni**
- 9:12 Paper 625e: Investigating the Concurrent Effect of Encapsulation and Perfusion on Chondrogenic Differentiation of Mesenchymal Stem Cells
- **Amin Vossoughi Shahvari**, Howard W. T. Matthew
- **9:30** Paper 625f: Bioadhesive Hydrogels with Antimicrobial and Osteoinductive Properties for Periodontal Applications
- Ehsan Shirzaei Sani, Aline Yaghsezian, Zheng Cao, Makiko Ishii, Nooshin Zandi, Giuseppe Intini, Flavia Pirih, Nasim Annabi
- **9:48** Paper 625g: Eggshell Particle-Reinforced Hydrogels for Bone Tissue Engineering
- Gulden Camci-Unal
- **10:06 Paper 625h:** Design of a Two-Phase System for the Sustained Delivery of Growth Factors for Bone Tissue Engineering Applications
- **Mariya Shevchuk**, Angela Wagner, Tinke-Marie De Witte, Camila Parra, Nicholas A. Peppas

(626) Biomaterials for Drug Delivery: Controlled Release

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Celebration 14
Matthew Webber, Chair
Mathumai Kanapathipillai, Co-Chair
Sutapa Barua, Co-Chair
Forrest Kievit, Co-Chair

Sponsored by: Biomaterials

- **8:00 Paper 626a:** Electrostatic Complexation of Insulin and Polycations As Glucose-Responsive Delivery Systems
- **Lisa R. Volpatti**, Delaney M. Burns, Arijit Basu, Robert Langer, Daniel G. Anderson
- **8:18 Paper 626b:** Design of a Slow-Releasing Antioxidant Drug Delivery System for Stroke
- **Nicholas Murphy**, Kyle Lampe
- **8:36** Paper 626c: Dual Growth Factor Delivery for Craniomaxillofacial Bone Repair Using Layer-By-Layer Technology *MayLin Howard*, *John Martin*, *Sheryl Wang*, *Paula T. Hammond*
- **8:54** Paper **626d**: Engineering Protein-Polymer Conjugates for Targeted Drug Delivery Applications
- Julia S. Kim, Allison R. Sirois, Analia J. Vazquez Cegla, Eugenie Jumai'an, Naomi Murata, Maren E. Buck, **Sarah** J. Moore
- **9:12** Paper **626e**: Design of pH-Responsive Hydrogels for Oral Delivery of High Isoelectric Point Therapeutic Proteins
- **Heidi F. Oldenkamp**, Isabel De La Fuente, Nicholas A. Peppas
- **9:30 Paper 626f:** Thermo-Sensitive Block Copolymers for the Local Delivery of Antibiotics
- Rong Yang, Daniel S. Kohane
- **9:48** Paper **626g**: Treating Obesity and Glucose Intolerance through Polymer Scaffold Delivery of Resveratrol to the Adipose Tissue
- **Michael Hendley**, Kendall Murphy, Christopher Isely, Prakasam Annamalai, Michael Gower
- **10:06** Paper **626h**: Formulation for Weeklong Oral Drug Delivery in a Gastric Resident Oral Dosage Form
- Rosemary Kanasty, Susan Low, Junghoon Yang, Saumya Moorthy, Erick Peeke, Marlene Schwarz, Juan Jaramillo Montezco, David Altreuter, Wright Jim, Tyler Grant, Andrew Bellinger, Alisha Weight

(627) Biomedical Applications of Protein Engineering Thursday, Nov 14, 8:00 AM

Hyatt Regency Orlando, Celebration 3 Jin Ryoun Kim, Co-Chair Kevin Metcalf, Co-Chair Robert Pantazes, Co-Chair

Sponsored by: Bioengineering

- **8:00 Paper 627a:** Engineering Multi-Epitopic Antibodies for Receptor Downregulation
- **Seth Ludwig**, Rakeeb Kureshi, Jamie B. Spangler
- **8:18** Paper 627b: Phi a Parameter for Quantifying the Specificity of Post-Translational Modification Site Targeting Antibodies
- Yongku Cho, Dan Li
- **8:36** Paper 627c: Engineering a Blue Light Inducible Spycatcher System (BLISS) As a Tool for Protein Photo-Patterning and Optogenetics
- **Emily Hartzell**, Justin Terr, Wilfred Chen
- **8:54** Paper **627d:** Amyloid Aggregation of *Bacillus Circulans* Xylanase Under Native Conditions and Its Modulation By β-Amyloid-Derived Peptide Fragments
- Timothy Charlton, Vandan Shah, Tonianna Lynch, Jason Candreva, Edward Chau, Yanxi Yang, Hyunjoo Kim, Amy Wood, **Jin Ryoun Kim**
- **9:12** Paper 627e: Optimizing Cell-Free Protein Synthesis for Increased Yield, Solubility and Activity of Antimicrobial Protein Colicins
- **Xing Jin**, Weston Kightlinger, Seok Hoon Hong
- **9:30** Paper 627f: Doxycycline Dependent Self-Inactivation of CRISPR-SpCas₉ to Temporally Regulate on- and Off-Target Editing
- Anju Kelkar, Yuqi Zhu, Theodore Groth, Gino Stolfa, Aimee Stablewski, Michael Nemeth, Naina Singhi, **Sriram Neelamegham**
- **9:48 Paper 627g:** A Platform Technology for Dynamic Control of Cell Behavior
- Laura Segatori

(628) Bionanotechnology for Gene and Drug Delivery I

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Discovery 45 Joo-Youp Lee, Chair Piyush Jain, Co-Chair

Sponsored by: Bionanotechnology

- **8:00 Paper 628a:** Magnetic Particle Imaging for In Vivo Quantitative Tracking of Nanoparticle Drug/Gene Carriers
- Carlos Rinaldi
- **8:40 Paper 628b:** pH-Responsive, Core-Shell Magnetite-Silver Nanoparticles for the Guided Transport and Delivery of Nucleotide Cargoes: An Avenue for Highly-Targeted Gene Therapies
- Carlos Manuel Ramirez Acosta, Juan C Cruz, Luis H. Reyes
- **8:58 Paper 628c:** Folate Receptor-Targeted Anionic Ternary Polyplexes for Gene Delivery
- Caleb Akers, Daniel W. Pack
- **9:16 Paper 628d:** Nanoparticle Carrying T Cells for Targeted Drug Delivery
- **Muhammad Raisul Abedin**, Yongjian Liu, Sutapa Barua

- 9:34 Paper 628e: Evaluating
 Toxicology, Immunogenicity, BioDistribution, and Pharmacokinetics of
 DNA Origami Nanostructures In Vivo
 Christopher R. Lucas, Patrick D.
 Halley, Amjad Chowdhury, Aparna
 Lakshmanan, Bonnie K. Harrington,
 Ronni Wasmuth, Larry Beaver, Rosa
 Lapalombella, Amy J. Johnson, Erin K.
 Hertlein, John C. Byrd, Carlos E. Castro
- **9:52** Paper 628f: From Fabrication to Characterization of Sucrose Microneedles with Dissolvable Polymers for Vaccine Delivery Systems
- **Mohammad Mofidfar**, Sanghyun Park, Walter E. Henderson, Amir Hejri, Mark R. Prausnitz
- **10:10** Paper **628g:** Rational Selection of Intestinal Permeation Enhancers for Oral Macromolecular Drug Delivery *Katherine Fein, Kathryn A. Whitehead*

(629) Catalysis for Biomass Upgrading I: Reaction Fundamentals

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Florida
Ballroom B
Jeremy S. Luterbacher, Chair
Zhenglong Li, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper **629a**: Predicting an Optimal Oxide/Metal Interface Catalyst for Hydrodeoxygenation Chemistry of Biomass Derivatives
- Shyam Deo, Michael Janik
- **8:18** Paper 629b: Developing Multi-Scale Models of Deoxygenation Reactions on Iron Carbide Catalysts: Hydrodeoxygenation of Phenol on Fe,C (001)
- **Neeru Chaudhary**, Jacob Bray, Renqin Zhang, Yong Wang, Jean-Sabin McEwen
- **8:36** Paper **629c:** Unravelling the Oxidative Coupling of Methanol on Au(111) Using First-Principles-Based Kinetic Modelling
- Romain Reocreux, Ioanna Fampiou, Michail Stamatakis
- **8:54** Paper **629d:** Brønsted Acid Sites on Tungsten Oxide/Platinum Catalysts *Shizhong Liu, Jiayi Fu, Weiqing Zheng, Stavros Caratzoulas, Dionisios G. Vlachos*
- **9:12** Paper 629e: Hydrodeoxygenation over Ptwox Catalysts: Isotopic Labeling *Kyle Stephens, Alan Allgeier*
- **9:30** Paper **629f**: Effect of Metal Chlorides on Glucose Mutarotation and Implications on Humin Molecular Structure
- Pranav Ramesh, Athanasios Kritikos, **George Tsilomelekis**
- **9:48** Paper **629g**: Kinetic Modeling of Ethanol Oligomerization over Calcium Hydroxyapatite
- **Nathaniel Eagan**, Michael Lanci, George W. Huber

10:06 Paper **629h:** Investigating the Origins of Selectivity Toward Maleic Anhydride during the Oxidation of Levulinic Acid over Supported Vanadium Oxides — *Ran Zhu, Anargyros Chatzidimitriou, Bowei Liu, Jesse Q. Bond*

(630) Catalytic Hydrocarbon Processing I: Methane

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom E Nan Yi, Chair Brett Loveless, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 630a: Catalytic Methane Decomposition in Molten KCI-MnCl₂ for the Co-Production of Hydrogen and Separable Graphitic Carbon

— Dohyung Kang, Nazanin Rahimi, Michael Gordon, Horia Metiu, **Eric McFarland**

8:20 Paper 630b: The Production of CO₂-Free Hydrogen and Carbon Materials By Methane Decomposition: Self-Sustained Production without Using Externally Added Catalyst

— I-Wen Wang, Jianli Hu

8:40 Paper 630c: Nickel-Based Dry Reforming Catalysts Modified By Atomic Layer Deposition: Effect of Reaction Conditions on ALD Films & Measuring Deactivating Catalysts at Isoconversion — Patrick Littlewood, Dingdi Wang, Eric Weitz, Peter C. Stair, Tobin J. Marks

9:00 Paper 630d: Insights into the Most Ideal Surface Chemistry for CH₄ Dry Reforming from Oxide-Supported Intermetallic Compound Nanoparticles of Well-Defined Bulk and Surface Composition

— **Max Mortensen**, Yuanjun Song, Yang He, Siris Laursen

9:20 Paper 630e: Oxidative Coupling of Methane Using Layered, Ruddlesden–Popper (R-P) Oxides — *Bingwen Wang, Eranda Nikolla*

9:40 Paper 630f: Shared Space: Interactions between Metal Cations in Cu/Zn-ZSM-5 Systems

- Zachary T. Gentle, Daniel F. Shantz

10:00 Paper 630g: Methane Activation over Mn/Na₂WO₄/SiO₂: The Balance of Surface Defects and Activated Oxygen Species

— **Yixiao Wang**, Zongtang Fang, Rebecca Fushimi, Gregory Yablonsky, M. Ross Kunz, Rakesh Batchu

(631) Characterization of Adsorbent Materials

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Manatee Spring II

Federico Brandani, Chair

Sponsored by: Adsorption and Ion Exchange

8:00 Paper 631a: Textural Characterization of Shale Nanostructure — Katie A. Cychosz, Enzo Mangano, Andrew E. Pomerantz, Stefano Brandani, Matthias Thommes

8:20 Paper 631b: Surface Area Determination of Metal-Organic Frameworks (MOFs) Using the Brunauer-Emmett-Teller (BET) Method: Limitations and Improvements

— **Archit Datar**, Priya Sinha, Chungsik Jeong, Xuepeng Deng, Yongchul G. Chung, Li-Chiang Lin

8:40 Paper 631c: Pore Size Estimation from Ultrasonic Measurements during Nitrogen Adsorption Experiment

— Max Maximov, Gennady Gor

9:00 Paper 631d: A Hydrogen-Bonded Supramolecular Coordinating Complex for Copper Removal from Aqueous Solutions with Unprecedentedly Fast Kinetics

— **Ngoc Bui**, Hyungmook Kang, Jeffrey J. Urban

 $\begin{array}{l} \textbf{9:40 Paper 631f:} & \text{Optimized Activation} \\ \text{of MIL-100Cr for Highly Efficient CO}_2 \\ \text{Capture and N}_2\text{O Removal} \\ \end{array}$

— Jiangfeng Yang

10:00 Paper 631g: Shape-Selective Adsorption Separation of C₄ Olefins in Gallate-Based Metal-Organic Frameworks

— **Jie Chen**, Zongbi Bao, Jiawei Wang, Zhiguo Zhang, Qiwei Yang, Yiwen Yang, Baogen Su, Qilong Ren

(632) Confluence of Experimental and Theoretical Methods

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom F Viktor J. Cybulskis, Chair Jean-Sabin McEwen, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 632a: How Advancements in Theory and Experiment Enabled the Synthesis of the First Enantiomerically Enriched, Polycrystalline Molecular Sieve — *Mark E. Davis*

8:40 Paper 632b: Spectroscopic and Kinetic Assessment of Brønsted Acid Site Proximity in Chabazite Zeolites

— **Philip M. Kester**, Jerry Crum, Sichi Li, William F. Schneider, Rajamani Gounder

9:00 Paper 632c: Kinetic Investigations of Carbonyl Reduction over Group VIII Metals: Acetone Hydrogenation

— Xin Gao, Andreas Heyden, **Omar A. Abdelrahman**, Jesse Q. Bond

9:20 Paper 632d: Hydrodeoxygenation of Phenolics at Solvent-Metal Interfaces: Enabling New Catalytic Pathways By Modifying the Reactive Hydrogen Species

— Alyssa Hensley, Junnan Shangguan, Jacob Bray, Matthew Gradiski, Robert Morris, Jean-Sabin McEwen, Ya-Huei (Cathy) Chin 9:40 Paper 632e: Dehydroaromatization of Ethylene over Metal-Exchanged H-ZSM-5 Catalysts: The Nature and Role of (Extra) Framework Acid Sites

— **Yunwen Zhou**, Hari Thirumalai, Lars C. Grabow, Jeffrey D. Rimer

10:00 Paper 632f: Not All Hydrogens Are Created Equal: Theoretical and Experimental Insight into How Protons and Hydrides Steer Different Hydrogenation Rates for Alkynes and O₂ over Au/TiO₂

— Sravan Kumar Kanchari Bavajigari, Todd Whittaker, James Bruno, Bert D. Chandler, Lars C. Grabow

(633) Control and Optimization of Particle and Solid Production

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 20 Heather N. Emady, Chair Bryan J. Ennis, Co-Chair

Sponsored by: Particle Production and Characterization

8:00 Paper 633a: Controllable Preparation of Uniform Magnesium Ethoxide Particles: The Effects of *N*-Hexane and Silicone Oil and Their Synergic Effect

— **Zhou Lan**, Lu Yangcheng

8:25 Paper 633b: Multi-Objective Optimization of Simple Crystallization Systems

— **Hao-Jen Pan**, Yu-Ti Tseng, Jeffrey D. Ward

8:50 Paper 633c: Scalable Fabrication of Multielement Ceramic Oxide Particles By an Aerosol Process

— **Yujia Liang**, Joseph A. Libera

9:15 Paper 633d: Controlling the Internal Structures of Polymeric Microspheres Via the Introduction of a Water-Soluble Organic Solvent

— **Yanping He**, Yanlin Sun, Delong Xie, Linhua Zhu

9:40 Break

10:05 Paper **633f:** Experimental and Numerical Study of a Radial Multi-Zone Vortex Chamber Spray Dryer

— Thomas Tourneur, Axel de Broqueville, Anton Sweere, Albert Poortinga, Anton Wemmers, Umair Jamil Ur Rahman, Artur Pozarlik, **Juray De Wilde**

(634) CO₂ Industrial, Engineering and R&D Approaches

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Blue Spring I/II
Kevin C. Leonard, Chair
Gonzalo Guillén-Gosálbez, Co-Chair

Sponsored by: Sustainability

8:00 Paper 634a: Amine-Based CO₂ Capture Aided By Acid/Base Catalyst: Advancement of Amine Regeneration Using Fe-MCM-41 Catalyst

— **Xiaowen Zhang**, Hongxia Gao**, Zhiwu Liang**, Paitoon Tontiwachwuthikul, Maohong Fan **8:18** Paper 634b: Enhancing Divalent Cation Rejection in Membrane Systems for the Treatment and Utilization of High Ionic Strength Waste Streams

— **Steven Bustillos**, Stephanie Aguilar, Abdulaziz Alturki, Erika Callagon La Plante, Richard Kaner, Dante Simonetti, Gauray Sant

8:36 Paper 634c: High Regeneration Efficiency and Low Viscosity of CO₂ Capture By Functionalized Ionic Liquid Organic Solution

— Fan Liu

8:54 Paper 634d: Understanding the Behavior of Degraded Amine Products on CO₂ Capture in Aqueous Amines By Molecular Simulations

— Cristina G. Martinez, Daniel Bahamon, Fèlix Llovell, **Lourdes F. Veaa**

9:12 Paper 634e: Ptmgfe/Ni-Based Al₂O₃-CeO₂ Catalysts for Dry-Reforming of Methane

— **Abbas Jawad**, Fateme Rezaei, Ali Rownaghi

(635) Design and Operations Under Uncertainty

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 25 Ali Mesbah, Chair Matthew D. Stuber, Co-Chair

Sponsored by: Systems and Process Design

8:00 Paper 635a: A Scalable Stochastic Programming Approach for Designing Flexible Systems

— Joshua Pulsipher, Victor M. Zavala

8:19 Paper 635b: Design Centering Problem through Flexibility Analysis Concepts

— **M. Paz Ochoa**, Anuja Deshpande, Stephen D. Stamatis, Salvador García-Muñoz, Ignacio E. Grossmann

8:38 Paper 635c: Data-Driven Feasibility Analysis for Modular Design Under Demand Variability

— Lisia S Dias, Athary Bhosekar,

Marianthi lerapetritou

8:57 Paper 635d: Robust Simulation of Transient PDE Models Under Uncertainty — *Chenyu Wang, Matthew D. Stuber*

9:16 Paper **635e**: Parametric & Adjustable Robust Optimization for the Integration of Design and Operation — *Styliani Avraamidou*, *Efstratios N. Pistikopoulos*

9:35 Paper 635f: A Multistage Stochastic Optimization Approach to Power Plant Scheduling with Flexible Carbon Capture

— **Manali S. Zantye**, Akhil Arora, M. M. Faruque Hasan

9:54 Paper **635g**: Robust Optimization for Chemical Process Design and Applications to Carbon Capture Technology

— **Natalie M. Isenberg**, Paul Akula, Debangsu Bhattacharyya, David C. Miller, Chrysanthos E. Gounaris

- **10:13 Paper 635h:** Optimal Scheduling of an Air Separation Unit for Demand Response Under Price and Demand Uncertainty
- **Morgan Kelley**, Ross Baldick, Michael Baldea

(636) Developments in Shale Oil, Oil Sands and Other Heavy Fuels

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Challenger 38/39

Seiya Hirohama, Chair Nevin Gerek, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

8:00 Paper 636a: Limitations on the Residual Solvent Recovery Imposed By the Gangue Characteristics

— Reza Khalkhali, Phillip Choi

8:25 Paper 636b: Estimation of Phase Equilibrium for Water-Heavy Oil System with Structural Information of Heavy Oil Components

— **Shogo Teratani**, Keita Katano, Tsutomu Nakamura, Soma Sato, Hiroshi Inomata

8:50 Paper 636c: Recovery of Heavy Hydrocarbons from Indonesian Asphalt Rocks through Solvent Extraction

— **Guoqiang Ma**, Hong Sui, Lin He, Xingang Li

9:15 Paper 636d: Chemical Kinetic Modeling Study of Heavy Hydrocarbons in Naturally Fractured Reservoirs through in-Situ Upgrading Technology

— **Jose Duran Armas**, Carlos Scott, Lante Carbognani, Pedro Pereira-Almao

9:40 Paper **636e:** Switchable-Hydrophilicity Triethylamine:Formation and Synergistic Effects of Asphaltenes in Stabilizing Emulsions Droplets

— **Jinjian Hou**, Xingang Li, Hong Sui, Lingyu Sun, Lin Xu

10:05 Paper 636f: Nanoscale Static and Dynamic Behavior and Optimized Controlling Technology of Gas Channeling in Shale Oil Reservoirs

— Kaiqiang Zhang, Songyan Li, Na Jia

(637) Distributed Chemical and Energy Processes for Sustainability

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Regency Ballroom U Carole Read, Chair

Nick AuYeung, Co-Chair Shweta Singh, Co-Chair

Sponsored by: Sustainable Energy

8:00 Paper 637a: Building Momentum for Sustainable Behaviors in Developing Regions Using Locally Managed Decentralized Circular Economy Principles

— **Jeffrey R. Seay**, Chandni Joshi

8:25 Paper 637e: Supply Chain Optimization of a Locally-Managed Decentralized Solution for Conversion of Waste Plastic to Fuel in Developing Regions

— Chandni Joshi, Jeffrey R. Seay

8:50 Paper 637c: Thermochemical Energy Storage Integration with Thermoelectric Power Generation
— Renuka Bhatt, Griffin S. Drake, Nick

9:15 Paper 637d: Techno-Economic Analysis and Life Cycle Assessment of Decentralized Preprocessing System for Fast Pyrolysis Biorefineries with Blended Feedstocks in the Southeastern USA

— Kai Lan, Longwen Ou, Sunkyu Park, Stephen S. Kelley, Burton C. English, Yuan Yao

9:40 Paper **637b**: Ammonia Decomposition to Produce Hydrogen Using Chemical Looping Approaches: Considerations and Results for High Pressure Operation

— **Mandar Kathe**, Deven Baser, Michael Petrecca, L.-S. Fan

(638) Drug Delivery I

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Celebration 2 Srivatsan Kidambi, Chair Greg Thurber, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

8:00 Paper **638a:** Solid Lipid Nanoparticles Based Protein Delivery Platform for Effective Non-Viral Gene Editing

— Jie Li, Niren Murthy

8:18 Paper 638b: Endocytosis Controls siRNA Efficiency and Cell Specific Targeting

— **Daniel Vocelle**, Christina Chan, S. Patrick Walton

8:36 Paper 638c: Design of Hybrid Polymer/Adenoviral Gene Delivery Vectors

— Yasmine Gabal, Joshua D. Ramsey

8:54 Paper 638d: Raltitrexed/ Hyaluronic Acid Coated Nanoparticles

for Chemoradiation of Colorectal Cancer
— Justin Rosch, Madeleine Landry,
Conroy Sun

9:12 Paper 638e: Reverse Perfluorocarbon Emulsions for Pulmonary Drug Delivery: Effects of Emulsion Formulation on Drug Mass Transfer

— **Diane L. Nelson**, Keith E. Cook, Robert D. Tilton

9:30 Paper 638f: Nanoparticle-Coated Floss for Treatment of Periodontitis

— **Seth Boese**, Harvinder Gill

9:48 Paper 638g: Invited: Engineering Macromolecular Oligotea Conjugates for Biological Applications

— Christopher A. Alabi

(639) Electrocatalytic Activation and Conversion of N2, NH3, and CO₂

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom D Gang Wu, Chair Adam Nielander, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 639a: New Insights into Electrochemical Ammonia Oxidation on Transition Metals from First Principles — *Hemanth S. Pillai*, *Hongliang Xin*

8:18 Paper 639b: Electrochemical Nitrogen Reduction Reaction: Quasi-Reference Electrodes for Improved Parameter Control

— **Benjamin L. Sheets**, Gerardine G. Botte

8:36 Paper 639c: Trends in the Electrocatalytic Nitrate Reduction Reaction across Transition Metals

— Jin-Xun Liu, Danielle Richards, Nirala

Singh, Bryan R. Goldsmith

8:54 Paper 639d: Nature of the First
Electron Transfer in Electrochemical
Ammonia Activation in a Nonaqueous

Medium
— Zachary Schiffer, Nikifar Lazouski,
Nathan Corbin, Karthish Manthiram

9:12 Paper 639e: The Role of Metal Nitrides in Selective Electrochemical Ammonia Synthesis

— **Michael Statt**, Aayush R. Singh, Brian A. Rohr, Jay Schwalbe, Matteo Carqnello, Jens K. Nørskov

9:30 Paper 639f: Understanding Ionic Liquid Assisted Selective CO₂ Reduction over Bi Metal Catalyst

— **Sahithi Gorthy**, Matthew Neurock, Joel Rosenthal

9:48 Break

10:06 Paper 639h: Investigation of Vapor-Fed Carbon Dioxide Reduction at the Solid Electrolyte-Catalyst Interface Using Zero-Gap Membrane Electrode Assemblies

— **Dong Un (Daniel) Lee**, Kabir Abiose, David Koshy, Christopher Hahn, Thomas F. Jaramillo

(640) Enabling and Advancing Formulations in Drug Product

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Celebration 6
Brendon G. Ricart, Chair
Mehrdad Kheiripour, Co-Chair
Xue (Ida) Chen, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 640a: Possible Synergistic Effects of Binary Polymers in Enhancing Release of a Poorly Soluble Drug from Amorphous Solid Dispersions

— Mahbubur Rahman, Alexander Coelho, Stephanie Ahmad, James Tarabokija, Sayali Bhujbal, Keanu Radaman, **Ecevit Bilgili**

8:18 Paper 640b: Modeling Fluidized Bed Impregnation of Active Pharmaceutical Ingredients Onto Porous Excipients

— Benjamin Glasser, Fernando Muzzio, **Plamen Grigorov**

8:36 Paper 640c: The Interaction of Solvent and Hypromellose Acetate Succinate Relate to Pharmaceutical Spray Dried Dispersion

— Daniel Burnett, **Jin Zhao**

8:54 Paper 640d: Effect of Preparative Methods on the Polymorph Found in Crystalline Solid-Dispersions of Flufenamic Acid

— Karina Sanabria Ortiz**, José Hernández Espinell**, Vilmalí López-Mejías, Torsten Stelzer

9:12 Paper 640e: Methodology to Rapidly Screen Lyophilization Formulations

- Christopher J. Morrison

9:30 Paper 640f: Towards Modelling the Morphology of Particles Obtained from Spray Dried Droplets

— **Hassan Abdullahi**, Christopher L. Burcham, Thomas Vetter

9:48 Paper 640g: Prediction of the Solubility of Active Pharmaceutical Ingredients Using the SAFT-γ Mie Group Contribution Approach

— **Malak Wehbe**, Sara Febra, Spiros Kournopoulos, George Jackson, Claire S. Adjiman, Amparo Galindo

10:06 Paper 640h: Predicting the Stability of Biotherapeutics in Liquid and Solid Formulations

- Sarah Hedberg, Daryl Williams

(641) Green Chemical Reaction Engineering for Sustainability

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Florida Ballroom A

Samuel Marre, Chair Wan-Ting (Grace) Chen, Co-Chair Miguel Modestino, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

8:00 Paper 641a: Autocatalysis in Surfactant Systems: Kinetics & Model of Tertiary Amine Oxidation in Water — Arnab Chaudhuri, Wyatt Winkenwerder, John van der Schaaf

8:22 Paper 641b: Cyclodextrins As Mass Transfer Agents for Au-Pd Nanoparticle Catalyzed Selective Oxidation Reaction of Methane in a Microfluidic Flow System

— Filip Popovic, Ryan L. Hartman

8:44 Paper 641c: Fundamentals of Multiphase Reaction Engineering for CO₂ Free Hydrogen Production from Natural Gas

— **Luke Minardi**, Faisal Alshafei, Dante Simonetti

9:06 Paper 641d: Synergism of Subcritical H₂O and Supercritical CO₂ for Glucose Conversion to 5-Hydroxymethylfufural

— Armando T. Quitain, Ryuto Inoue, Samantha Siew, Yeo Jhin Xern, Yik Lam Kam, Jonas Karl N. Agutaya, Mitsuru Sasaki, Maria Jose Cocero, Tetsuya Kida

9:28 Paper **641e**: The Use of Sand As Sustainable Catalyst in H₂ Production from NaBH₄ Methanolysis
— Sahin Demirci, Aydin K. Sunol,

— Sanin Demirci, Ayain K. Suno. **Nurettin Sahiner**

9:50 Paper 641f: Sustainability Study on Point of Use Scrubber Canister Used in Semiconductor Industry

— Vivian Hui

10:12 Paper 641g: Continuous Membrane Reactors for Asymmetric Synthesis and Separation in Organic Media

Levente Cseri, Peter Kisszekelyi,
 Abdulaziz Alammar, Jozsef Kupai,
 Gyorgy Szekely

(642) In-Silico Tools for Accelerating Pharmaceutical Process Development

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Celebration 7 Kushal Sinha, Chair Qinglin Su, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

8:00 Paper 642a: Two-Phase Optimal Design of Pharmaceutical Separation: Sampling-Based Uncertainty Analysis and Reinforcement Learning

— **Soonho Hwangbo**, Gürkan Sin

8:17 Paper 642b: Computer-Aided Design of Solvent Blends for the Cooling and Anti-Solvent Crystallisation of Active Pharmaceutical Ingredients

— **Oliver L. Watson**, Amparo Galindo, George Jackson, Claire S. Adjiman

8:34 Paper 642c: Two-Dimensional Moisture Content and Size Evolution during Fluid Bed Drying As Part of a Continuous Pharmaceutical Manufacturing Process Using NIR-CI

— **Michael Ghijs**, Brecht Vanbillemont, Niels Nicolaï, Michiel Peeters, Thomas De Beer, Ingmar Nopens

8:51 Paper 642d: Continuous Mixing Technology: Design Space Exploration with Discrete Element Simulations

— **Peter Toson**, Pankaj Doshi, Eva Siegmann, Johannes G. Khinast, Daniel O. Blackwood, Ashwinkumar Jain, Alexandre Bonnassieux, Dalibor Jajcevic

9:08 Paper **642e:** Validation of Combined PBM-RTD Technique to Simulate Continuous Wet Granulation Systems for Pharmaceutical Manufacturing Processes

— **Shashank V. Muddu**, Rohit Ramachandran

9:25 Paper 642f: Computational Modeling of Liposome Formation in a Continuous Jet Flow Process Using CFD and MD

— **Hossein Mohammadiarani**, Antonio Costa, Xiaoming Xu, Su-Lin Lee, Celia N. Cruz, Diane Burgess, Bodhisattwa Chaudhuri

9:42 Paper 642g: A Big Data Analytics Workflow for Pharmaceutical Manufacturing Industry

— **Sheng Zhang**, Xinyuan Xie, Haibin Qu **9:58** Paper 642h: An Efficient Data-Based Methodology to Identify the Design Space of Continuous Pharmaceutical Manufacturing Processes

— **Nirupaplava Metta**, Marianthi Ierapetritou, Rohit Ramachandran

10:14 Paper 642i: Condition Based Maintenance for Sensor Network Reliability in Continuous Oral Solid Dose Manufacturing

— **Sudarshan Ganesh**, Benjamin Rentz, Qinglin Su, Francesco Rossi, Zoltan K. Nagy, G. V. Rex Reklaitis

(643) Ionic Liquids: Properties and Thermodynamics

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Regency Ballroom Q

Kevin N. West, Chair Suojiang Zhang, Co-Chair Dickson E. Ozokwelu, Co-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 643a: Thermal Stability of Imidazolium-Based Ionic Liquids: The Effects of Alkyl Chain Length, Environment, and Heating Conditions — *Michael Williams, Erdogan Kiran*

8:18 Paper 643b: Thermodynamics of the Mixtures of Ammonia and Ionic Liquids

— **Tugba Turnaoglu**, Mark B. Shiflett

8:36 Paper 643c: Characterization of 1-Ethyl-3-Methyl-Imidazolium Ionic Liquid Behavior in Non-Aqueous Solvents

— **Oscar Nordness**, Andres Miranda, Joan F. Brennecke

8:54 Paper 643d: Investigation of Ion Correlations in Ionic Liquid and Organic Solvent Mixtures through Scalable Screening

— **Ray Matsumoto**, Matt Thompson, Peter T. Cummings

9:12 Paper **643e**: *In Situ* Grazing-Incidence Wide Angle X-Ray Scattering (GIWAXS) Investigation of Effects of Silica Nanopore Confinement on Crystallization of [BMIM] Ionic Liquids

— Yuxin He, Joshua Garay, M. Arif Khan, Aniruddha Shirodkar, Joseph Strzalka, Folami Ladipo, Barbara L. Knutson, Stephen E. Rankin, Stephen Goodlett

9:30 Paper 643f: Impact of Carbon Number of Carboxylic Acid on the Polarity of Hydrophobic Deep Eutectic Solvent

— Kyle McGaughy, M.Toufiq Reza

9:48 Paper 643g: The Effect of Cation Polarity on the Melting Points of Ionic Liquids: An Experimental and Computational Study

— **Brooks D. Rabideau**, Mohammad Soltani, E. Alan Salter, Andrzej Wierzbicki, Kevin N. West, James H. Davis Jr. **10:06** Paper **643h**: Change Regulation of Cellulose Depolymerization during Dissolving Process in Ionic Liquids — *Fengjiao Pan*, *Le Zhou, Zhaoqing Kang, Yi Nie, Xiangping Zhang, Suojiang Zhang*

(644) Lithium and Beyond: Fundamental Advances in High Performance Batteries I

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Plaza International Ballroom I Robert J. Messinger, Chair Lauren Marbella, Co-Chair

Sponsored by: Electrochemical Fundamentals

8:00 Paper 644a: Improved Understanding of the Role of Ultra-Thin ALD Films on Lithium Metal Oxide Cathode Materials

— Amanda Hoskins, Samantha L. Millican, Tyler Gossett, Yan Gao, Xinhua Liang, Charles B. Musgrave, **Alan W**.

8:20 Paper 644b: Operando Studies to Enumerate the Electrochemical Phase Transformations of MnO₂

— **Joshua W. Gallaway**, Sanjoy Banerjee, Gautam G. Yadav, Damon Turney

8:40 Paper **644i**: Insights into Li-Ion Battery Cathode Degradation from Atomic-Scale Modeling

— Alexander Urban

8:55 Paper 644d: Aluminum-Ion Transport and Charge Transfer Mechanism in Chevrel Phase Electrodes for Rechargeable Aluminum Batteries — Ankur Jadhay Leffrey Xu Robert I.

— **Ankur Jadhav**, Jeffrey Xu, Robert J. Messinger

9:10 Paper 644e: In Situ Characterization of the Lithium Metal Interface

— **Jeffrey Lopez**, Yang Shao-Horn

9:25 Paper 644f: Modeling the Interface between Lithium Metal and Its Native Oxide

— **Jeffrey S. Lowe**, Donald J. Siegel

9:40 Paper 644g: Nonpolar-Based Electrolytes for Improved Lithium Metal Deposition and Stripping

— **Chibueze Amanchukwu**, Yi Cui, Zhenan Bao

9:55 Paper 644h: Interfacial Origins of Degradation in High Energy Li-Rich NMC Cathodes Probed By Online Electrochemical Mass Spectrometry

— **Srini Ramakrishnan**, Byungchun Park, Lori Kaufman, Bryan D. McCloskey

10:10 Paper 644c: 7Li NMR Chemical Shift Imaging of Microstructural Growth of Lithium in All-Solid-State Batteries

- Lauren Marbella

(645) Manufacturing Process Improvements for Chemical/ Petrochemical Industries

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 18 Qiang Xu, Chair Honglin Qu, Co-Chair

Sponsored by: Technology Transfer and Manufacturing

8:00 Paper **645**a: Toll Manufacturing: A Sharing-Economy Model for on-Demand Chemical Production Services

— **Akhil Arora**, M. M. Faruque Hasan

8:25 Paper 645b: Integrated Process Development and Economic Evaluations for an Optimum Gas Processing Plant — *Mozammel Mazumder*, *Qiana Xu*

8:50 Paper 645c: Modeling of Skinning Effect and Optimization of Dry-Casting Process

— **Jaehyun Shim**, Sang Hwan Son, Jona Min Lee

9:15 Paper 645d: Investigations on the Dynamics and Mechanics of Milling Processes for Mechanochemistry

— Ciara Griffin, Patrick Cronin, Alan Ryan, Ahmad Albadarin, Gavin Walker

9:40 Paper 645e: Process Considerations to Maximize Catalyst Activity in Solution Polyolefin Polymerizations

- Aaron H. Reed

(646) Membrane-Based Organic Solvent Separations I

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Barrel Spring II
Ryan Lively, Co-Chair
Andrew Livingston, Co-Chair
Guanghui Zhu, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper **646a**: Nanoengineered Solvent-Resistant Membranes from Biophenols and Graphene

— Fan Fei, Jeong Kim, Gergo Ignacz, Hai Anh Le Phuong, Levente Cseri, Young Moo Lee, Christopher F. Blanford, **Gyorgy Szekely**

8:21 Paper 646b: Vapor-Phase Crosslinked Mixed Matrix Membranes with UiO-66-NH₂ for Organic Solvent Nanofiltration

— **Zhuo Fan Gao**, Yingnan Feng, Dangchen Ma, Neal Tai-Shung Chung

8:42 Paper 646c: Anti-Tradeoff Graphene Oxide Membrane for Organic Solvent Nanofiltration

- Shaofei Wang, Suzana P. Nunes

9:03 Paper 646d: Torlon® Hollow Fiber Membranes for Organic Solvent Reverse Osmosis Separation of Complex Aromatic Hydrocarbon Mixtures — Hye Youn Jang, Ryan Lively, JR

9:24 Paper 646e: Molecular Design of Polymeric Membranes with Tunable Gradient Pores for Organic Solvent Nanofiltration

— **Qi Shi**, Jianwen Jiang

Johnson, Dhaval Bhandari

- 9:45 Paper 646f: Novel Metal Organic Brush Membranes (MOBs) for Organic Solvent Nanofiltration
- **Pranav Ramesh**, Weiwei Xu, Miao Yu, Georges Belfort
- 10:06 Paper 646g: Two-Dimensional Molybdenum Disulphide Membranes for Organic Solvent Nanofiltration: Stability. Structural Manipulation and Separation Performances
- Shudong Jiang, Bingyi Guo**, Sui** Zhang
- (647) Modeling Approaches and Applications in Fluidization **Fundamentals**

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 19 Mikio Sakai, Chair Lev Davydov, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

- 8:00 Paper 647a: Spatially-Averaged Models for Moderately Dense Gas-Particle Flows Including a Thermal **Energy Balance**
- Stefanie Rauchenzauner, **Simon Schneiderbauer**
- 8:22 Paper 647b: Validating Optimal Drag Corrections for the Simulation of Sand Biomass Co-Fluidization
- Ligiang Lu, Xi Gao, Mehrdad Shahnam, William A. Rogers
- 8:44 Paper 647c: Particle-Scale Investigations of Reactive Fluidized Beds Based on CFD-DEM Coupling Methods
- Chenshu Hu, Kun Luo, Junjie Lin, Jianren Fan
- 9:06 Paper 647d: A Structural Model of Sub-Grid Drift Velocity for Fluidized Gas-Particle Flows
- **Ming Jiang**, Xiao Chen, Qiang Zhou
- 9:28 Paper 647e: A Cascading Approach to Develop a Filtered Drag Force Model for Large-Scale Gas-Particle Flows
- Yundi Jiang, Jari Kolehmainen, Ali Ozel, Sankaran Sundaresan
- 9:50 Paper 647f: Comparative Analysis of Drag Model Predictions for Fluidized **Bed Applications**
- Casey Q. LaMarche, Ben Freireich, Ray Cocco
- 10:12 Paper 647q: Numerical Modeling on Gas-Solid Two-Phase Flow Including Thin Plates
- Kazuya Takabatake, Mikio Sakai

(648) Molecular Simulation and **Modeling of Complex Molecules** Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Peacock Spring Yamil Colon, Chair Peng Bai, Co-Chair

Sponsored by: Thermodynamics and **Transport Properties**

- 8:00 Paper 648a: Atomistic Insight Towards the Effects of Conjugated Charged Polymers to α-Chymotripsin - Aravinda Munasinghe, Stefanie Baker, Ping Lin, Alan Russell, Coray M.
- 8:17 Paper 648b: Unraveling the Morphology of Melanin Nanoparticles Using Atomistic Molecular Dynamics
- **Utkarsh Kapoor**, Arthi Jayaraman
- 8:34 Paper 648c: Reactive Molecular Dynamics Simulation of Cellulose and Its Property Evolution Under Pyrolysis Conditions
- **Qi Qiao**, Liangliang Huang
- 8:51 Paper 648d: Computational Modeling and Simulation Studies on the Binding of Toxic Compounds to Montmorillonite Clay
- Shujun He, Asuka A. Orr, Meichen Wana, Sara E Hearon, Timothy D Phillips, Phanourios Tamamis
- 9:08 Paper 648e: Quantitatively Accurate Theory to Predict Adsorbed Configurations of Surfactants on Metal Surfaces
- Sumit Sharma
- 9:25 Paper 648f: Molecular Simulations of Corrosion Inhibitors on Metal Surface at Operating Conditions
- Seba Al-Areeqi, Hashir Nasim, Daniel Bahamon, Ricardo Noqueira, Lourdes F. Vega
- 9:42 Paper 648g: Effect of Electric Field on Competitive Associations in Zwitterionic Electrolytes: A Molecular Simulation Study
- **Manh Tien Nguyen**, Qing Shao
- 9:59 Break

10:12 Paper 648i: Meso-Scale Modeling in Gas-Solid Fluidizaton and Applications in Catalytic Fluidized Beds

Bona Lu

(649) Multifunctional Composites Thursday, Nov 14, 8:00 AM

Hyatt Regency Orlando, Celebration 11 John Zhanhu Guo, Chair Zhen Liu, Co-Chair Pinghua Ling, Co-Chair

Sponsored by: Composites

- 8:00 Paper 649a: Synergistically Enhancing Gas-Barrier and UV-Blocking Performance of Biodegradable Films Via Compositing with Aligned Graphene
- Jiaxu Li, Steven J. Severtson, Pingwei Liu, Wen-Jun Wang
- 8:25 Paper 649b: Expanding the Formulation Boundaries for Soft, Stretchable Liquid Metal Composites Amanda Koh
- 8:50 Paper 649c: Kirigami-Enabled, Passive Resonant Sensors for Wireless **Deformation Monitoring**
- Sadaf Charkhabi, Yee J. Chan, Doh-Gyu Hwang, Sean T. Frey, Michael D. Bartlett, Nigel Reuel

- 9:15 Paper 649d: Surface-Agnostic Highly Stretchable and Bendable Conductive Mxene/Polymer Multilayers for Sensing Applications
- Hyosung An, Touseef Habib, Smit Shah, Huili Gao, Anish Patel, Ian Echols, Miladin Radovic, Micah J. Green, Jodie L. Lutkenhaus
- 9:40 Paper 649e: Directed Printing and Reconfiguration of Thermoresponsive Silica-Pnipam Nanocomposites
- Yusheng Guo, Jorge Belgodere, Yingzhen Ma, Jangwook Jung, Bhuvnesh Bharti

(650) Nanomaterials for Biological Applications I

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Discovery 44 Cerasela Zoica Dinu, Chair Jaeyun Kim, Co-Chair

Sponsored by: Bionanotechnology

- 8:00 Paper 650a: Chiral Supraparticles for Controllable Nanomedicine - Jihyeon Yeom, Pedro Guimaraes, Michael J. Mitchell, Ana Jaklenec, Robert Langer
- 8:20 Paper 650b: Quantifying Nanoparticle Delivery to Solid Tumors at the Cellular Level
- Stefan Wilhelm
- 9:10 Paper 650c: Aloe Vera-Mediated Green Synthesis of Tellurium Nanostructures with Both Antimicrobial and Anticancer Activity
- Ada Vernet Crua, David Medina, Jorge Luis Cholula Diaz, Jose Miguel Garcia Martin, Thomas J. Webster
- 9:30 Paper 650d: Cancer Microtissues for Rationalized Nanoparticle Based Radiotherapy
- Anna Lena Neuer, Lukas Gerken, Kerda Keevend, Inge K. Herrmann
- 9:50 Paper 650e: Projection-Specific Modulation of Neural Activity with a Non-Genetic Method
- Huiliang Wang, Lief Fenno, Yunsheng Chen, Christina Kim, Charu Ramakrishnan, Masatoshi Inoue, Sanjiv Sam Gambhir, Karl Deisseroth
- 10:10 Paper 650f: Understanding and Controlling the Plant Antifungal Activity of New Classes of Environmentally Benian Nanoparticles
- Cathryn Conner, Aditya Sapre, Orlin
- (651) Particle Formation and **Crystallization Processes from Liquids, Slurries, and Emulsions** Thursday, Nov 14, 8:00 AM

Hyatt Regency Orlando, Coral Spring I/II **Thomas Vetter, Chair** Ryan C. Snyder, Co-Chair

Sponsored by: Crystallization and Evaporation

8:00 Welcoming Remarks

8:03 Break

- 8:24 Paper 651b: Toward Equant Shaped Crystal Habit through a 3-Stage Cyclic Process: Design and Applications - Pietro Binel, Fabio Salvatori, Marco
- 8:45 Paper 651c: A Quick Design of Spherical Agglomeration of Cefotaxime Sodium Based on Adhesion Free Energy - Xiaowei Cheng, Fei Li, Xin Huang, Hongxun Hao
- 9:06 Paper 651d: Impact of Polyvinylpyrrolidone (PVP) on the Polymorphism of Succinic Acid Formed Via Monodisperse Droplet Evaporation – Thaddeus Egnaczyk**, Ryan C.**
- 9:27 Paper 651e: Enhanced Nucleation at Liquid-Liquid Interfaces Due to Local Supersaturation
- David McKechnie, Saraf Zahid, Paul A. Mulheran, Jan Sefcik, Karen Johnston
- 9:48 Paper 651f: Emergence of Faceted Spiral Patterns during Eutectic Crystallization
- Saman Moniri, Hrishikesh Bale, Tobias Volkenandt, Yeqing Wang, Jianrong Gao, Tianxiang Lu, Kai Sun, Ashwin J. Shahani
- 10:09 Paper 651g: Characterization and Formation Mechanism of Crystal Defects of Drug a
- Lina Zhou, Yongli Wang, Zengrui Yu

(652) Particle Separations (Solid/ Solid, Solid/Liquid, Solid/Gas) Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 21 Gary Liu, Chair Richard M. Lueptow, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- 8:00 Paper 652a: Compressible Nutsche Cake Filtration - Retarding Effect of Residual Base-Cake
- Patrick McGough, Chris Chappelow, Madhusudhan Kodam
- 8:18 Paper 652b: Free Surface Profiles in Centrifuge Filtration at Low Speeds -Theoretical and Computational Solutions – Madhusudhan Kodam
- 8:36 Paper 652c: Developing Hollow Fiber Air Filters for Filtration of Ultrafine
- Liang-Yi Wang, Liya E Yu, Neal Tai-Shung Chung
- 8:54 Paper 652d: Cyclone Design and Performance at Restriced Space
- Ulrich Muschelknautz
- 9:12 Paper 652e: Self-Cleaning Electrostatic Oil Mist Collector By Using Corona Discharge and Surface Dielectric Barrier Discharge
- Myung Soo Kang, Jaeuk Shin, Jungho Hwang
- 9:30 Paper 652f: Optimization of Classifier Height and Nozzle Angle in a Jet Mill
- Mahesh Dhakate, Devang V. Khakhar, Jyeshtharaj B. Joshi

9:48 Paper 652g: Enhancement of Fluorite Flotation Process with the Combination of in-Situ Modification By Ball-Milling and Gas-Liquid Microdispersion

— Lu Ye

(653) Polymer Crystallization and Properties of Semi-Crystalline Polymers

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Celebration 12/13

Julie N. L. Albert, Chair Doug R. Tree, Co-Chair

Sponsored by: Polymers

- **8:00** Paper 653a: Suppression of Crystallization in Ultra-Thin and Thin Films of Cellulose Acetates and Their Blends and Its Effect on Gas Transport Characteristics
- **Hien Nguyen**, Ming-Yin Hsiao, Mengyuan Wang, Yifu Ding, Kazukiyo Nagai, Haiqing Lin
- 8:15 Paper 653b: Carefully Controlled Photo-Crosslinkable PLA Networks — Nicholas Baksh, Nathan Gallant, Ryan Toomey
- **8:30** Paper 653c: Structure-Processing-Property Relationships of 3-Hexylthiophene-Containing Statistical Copolymers
- **Michael Minkler Jr.**, Jihyuk Kim, Tucker Sparks, Bryan S. Beckingham
- **8:45** Paper **653d:** Crystallization-Driven Self-Assembly of Model Anisotropic Particles from Diblock Copolymers
- **Avanish Bharati**, Steven D. Hudson, Katie Weigandt
- **9:00** Paper 653e: Hierarchical Crystallization Processes in Double-Crystalline PEO-*B*-PCL Copolymers *Ryan M. Van Horn*
- **9:30** Paper 653f: Slip-Link Modeling of a Crystallizing Entangled Polymer Melt *Marat Andreev, Gregory C.* Rutledge
- **9:45** Paper **653g**: The Effect of Flow-Induced Fluctuations on Crystal Nucleation in the Polyethylene Melt *David A. Nicholson*, *Gregory C. Rutledge*
- **10:00 Paper 653h:** In Situ Formation of Zinc Phthalate As a Highly Dispersed β-Nucleating Agent for Mechanically Strengthened Isotactic Polypropylene *Shicheng Zhao*
- **10:15** Paper **653i**: In Situ Generation of a Self-Dispersed β -Nucleating Agent with Increased Nucleation Efficiency in Isotactic Polypropylene
- Qin Wei, Shicheng Zhao, Zhong Xin

(654) Polymer Reaction Engineering Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Celebration 5 Amy M. Peterson, Chair Wyatt Tenhaeff, Co-Chair

Sponsored by: Polymers

- 8:00 Paper 654a: Fluid Mechanics Meets Controlled Polymerizations: Theory, Experiments, and Beyond — Damien Guironnet, Dylan Walsh
- **8:30 Paper 654b:** N-Al Lewis Pair Catalysts for Functional-Group Tolerant Living Epoxide Polymerization
- Nathaniel A. Lynd, Robert C. Ferrier
 Jr., Christina G. Rodriguez, Jennifer
 Imbrogno, Malgorzata Chwatko
- 8:45 Paper 654c: Model-Based Synthesis of Ferrocene Microgels — Falco Jung, Sabine Schneider, Adel Mhamdi, Felix Plamper, Alexander Mitsos
- **9:00** Paper **654d:** Using Monomer Chemistry to Predict Dose Rate Effects during Electron Beam Polymerization *Nicole L. K. Thiher, Sage M. Schissel, Julie L. P. Jessop*
- **9:15** Paper 654e: Population Balances for Polymer Upcycling Processes: A Framework for Testing Mechanistic Hypotheses
- Ryan Yappert, Baron Peters
- **9:30** Paper 654f: Synthesis and Applications of Rapidly Degradable Polyphthalaldehyde Based Copolymers *Anthony Engler, Paul A. Kohl*
- **9:45** Paper 654g: An Efficient Process for the Cu(0)-Catalyzed Controlled Radical Synthesis and Subsequent Chain Extension of Poly(Methyl Acrylate) Macroinitiator
- Niloofar Shirali Zadeh, **Robin A. Hutchinson**
- **10:00 Paper 654h:** Preparation and Characterization of Dual-Branching Thermoplastic Polyolefin Elastomer Via a Tandem Solution Copolymerization System
- Kailun Zhang, **Donghui Bai**, Pingwei Liu, Wen-Jun Wang, Bo-Geng Li
- 10:15 Paper 654i: Model-Based Design and Synthesis of Copolymer Sequence Distributions through Programmed Semibatch RAFT Mini-Emulsion Copolymerization of Styrene and Butyl Acrylate
- Shiping Zhu, Bo-Geng Li, Wen-Jun Wang**, Jie Jiang**

(655) Process Engineering in Food and Bioprocess Industries

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Celebration 1
Nuttha Thongchul, Chair
Chuang Xue, Co-Chair
Jie Dong, Co-Chair

Sponsored by: Food

- **8:00** Paper 655a: Comparison of the Behavior and Distribution of Shear and Extension Rates in a Model Sigma Blade Mixer for a Non-Newtonian Fluid
- **Neslihan Bozdogan**, Sebnem Tavman, Seher Kumcuoglu, Jozef Kokini
- **8:18 Paper 655b:** 3D Time Variant Reactor Engineering Model for Red Wine Fermentations
- Konrad Miller, David E. Block 8:36 Paper 655c: In silico Metabolic

- Design of Two-Strain Bio Film Systems Predicts Enhanced Biomass Production and Biochemical Synthesis
- Ayushi Patel, **Michael A. Henson**, Ross P. Carlson
- **8:54** Paper **655d**: Strategies for Enhancing Glycerol Production in Yeast *Nuttha Thongchul, Sitanan Thitiprasert, Jesnipit Thammaket*
- 9:12 Paper 655e: Synthesis of Oligosaccharides Directly from Monoand Di-Saccharides As Potential Prebiotics in Inorganic Ionic Liquid — Ning Li, Jee-Hwan Oh, Jan Peter van Pijkeren, George W. Huber, Xuejun Pan
- **9:30 Paper 655f:** Bioprocess Development for High Cell Mass and Bioactive Antimicrobial Metabolites Production of *Lactobacillus Reuteri*
- **Hesham EL Enshasy**, Shanmugaprakasham Selvamani, Rajni Hatti-Kaul, Roslinda Abd Malek, Daniel Joe Dailin, Vijai Gupta
- **9:48** Paper 655g: Keynote: High Performance of Sugar Utilization to Produce D-Lactic Acid By Sporolactobacillus Terrae SBT-1
- **Sitanan Thitiprasert**, Jirabhorn Piluk, Vasana Tolieng, Somboon Tanasupawat, Nuttha Thongchul

(656) Process Intensification By Process Integration

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 17 Hannsjörg Freund, Chair Honglin Qu, Co-Chair Kumar Prashant, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

- **8:00 Paper 656a:** Carbonate Fuel Cells: Scaling-up the Magic Carbon Capture Box
- **Brandon O'Neill**, Rodrigo Blanco-Gutierrez, Keith E. Davis, Frank Dobek, Hossein Ghezel-Ayagh, Lu Han, Timothy M. Healy, Yesim Igci, Jonathan Rosen, Carl Willman, Wei Yang
- **8:25 Paper 656b:** Building Block-Based Work and Heat Exchanger Network Synthesis (WHENS)
- **Jianping Li**, Salih E. Demirel, M. M. Faruque Hasan
- **8:50 Paper 656c:** Photocatalytic Synthesis of Benzylic Amines Using Metal-Free Dyes: Investigating the Reaction Performance with a Spinning Disc Reactor and a Microchannel Reactor
- Alba Acevedo Fernandez, Shyam Rana, Duncan L. Browne, David R. Carbery, Emma Emanuelsson
- **9:15 Paper 656d:** Oxidation of L-Methionine in a Rotor-Stator Spinning Disc Reactor
- **Arnab Chaudhuri**, Koen Kuijpers, Parimala Shivaprasad, Emma Emanuelsson, Timothy Noel, John van der Schaaf

- **9:40 Paper 656e:** Development of Sorption Enhanced Reactive Processes for the Sustainable Production of Solketal through the Ketalization of Glycerol
- **Rui Faria**, Miguel Moreira, Ana M. Ribeiro, Alírio E. Rodrigues
- **10:05** Paper **656f**: Gradual Synthesis of Heat Exchanger Networks Under Economic, Environmental and Safety Considerations
- Arturo Jiménez-Gutiérrez, **Andrea Paulina Ortiz-Espinoza**, **Mahmoud**El-Halwaai

(657) PSE Methods for Safety and Reliability

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Bayhill 26 Costas Kravaris, Chair Iiro Harjunkoski, Co-Chair

Sponsored by: Computing Systems and Technology Division

- **8:00** Paper 657a: Integrated Redundancy, Storage and Maintenance Policy Design Optimization for Reliable ASU Based on Markov Chain a Game Theoretic Solution Approach
- **Yixin Ye**, Ignacio E. Grossmann, Jose M. Pinto, Sivaraman Ramaswamy
- **8:19 Paper 657b:** Incorporating Process Safety in Heat Exchanger Network Synthesis
- **Ahmed Harhara**, M. Sam Mannan, M. M. Faruque Hasan
- **8:38 Paper 657c:** Process Design and Control Interactions Under Time-Varying Operating Strategies
- **Henrique Oyama**, Helen Durand
- **8:57 Paper 657d:** Safety-Centered Process Control Based on Dynamic Safe Sets
- **Joshiba Ariamuthu Venkidasalapathy**, Costas Kravaris, M. Sam Mannan
- **9:15 Paper 657e:** Optimal Closest-Feasible-Points Non-Invariance Compensators
- Masoud Soroush
- **9:34 Paper 657f:** Operation Safety of Fluid Catalytic Cracking Process Via Model Predictive Control
- **Zhihao Zhang**, Carlos Garcia, David Rincon, Zhe Wu, Panagiotis D. Christofides
- 9:53 Paper 657g: Industrial-Scale Selective Maintenance Optimization Using Bathtub-Shaped Failure Rates — Teemu Ikonen, Hossein Mostafaei, Yixin Ye, Ignacio E. Grossmann, Iiro Hariunkoski
- **10:11** Paper **657h:** Data-Driven Estimation of Chemical Releases from End-of-Life Management Scenarios
- Jose D. Hernandez-Betancur, Gerardo J. Ruiz-Mercado, John P. Abraham, Wesley Ingwersen, Raymond L. Smith, David E. Meyer, Michael A. Gonzalez

(658) Rare Earth Elements: **Extraction, Separation,** Characterization, Economics, Criticality, and Kinetics

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Challenger 41/42

Evan J. Granite, Chair

Sponsored by: Advances in Fossil **Energy R&D**

8:00 Paper 658a: Recovery of Rare Earth Elements and Critical Materials from Coal and Coal-Based Resources

– Mary Anne Alvin

- 8:17 Paper 658b: Updates on the Bench-Scale Extraction and Concentration of Rare Earth Elements from North Dakota Lignite
- Nolan Theaker, Brittany Rew, Michael Mann, Steve Benson
- 8:34 Paper 658c: Identification of Optimum Coal Byproducts for Recovery of Rare Earths
- Evan J. Granite, Ward A. Burgess, Murphy J. Keller, Daejin Kim, Gordon Chiu

8:51 Break

- 9:08 Paper 658e: Effect of Acidity and Particle Size on the Kinetics of Leaching of Rare Earth Elements from Coal Ash
- Ward A. Burgess, Evan J. Granite, Murphy J. Keller, Bret H. Howard, Timothy Cain
- 9:25 Paper 658f: Utilizing Biooxidation in a Flow Sheet to Facilitate Low-Cost Rare Earth Elements Extraction from Coal-Based Resources and Eliminate Future Acid Mine Drainage
- Michael Free, Aaron Noble, Gerald
- 9:42 Paper 658g: Economic Extraction and Recovery of Rees and Production of Clean Value-Added Products from Low-Rank Coal Fly Ash
- Bruce Folkedahl, Carolyn Nyberg, R. Shane Addleman, Anthony Zinn
- 9:58 Paper 658h: Recovering Rare Earth Elements from Acid Mine Drainage Using Coal Combustion By-Products through Mine Reclamation
- Chin-Min Cheng, Jeffrey M. Bielicki, John Lenhart, Tarunit Butalia
- 10:14 Paper 658i: Membrane and Sorbent Based Recovery of Rare-Earth-Elements (REE) from Acid Mine Drainage Sludge
- Zachary Hendren, Mustapha Soukri, Elliot Reid, Gyu Dong Kim

(659) Recent Advances in Interfacial and Nano Particle Simulation Methods

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Rock Spring I/II Harold W. Hatch, Chair

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

8:00 Paper 659a: Rigid Seeding: A Computationally Efficient Method to Study Heterogeneous Nucleation in Molecular Simulations

— Tianmu Yuan**, Sapna Sarupria**, Ryan DeFever

- 8:30 Paper 659b: Theoretical and Computational Investigation of the Impact of Free Interfaces on Ice Nucleation
- Sarwar Hussain, Amir Haji-Akbari
- 8:45 Paper 659c: Evaluation of the Interface Potential Via a Force-Based Virtual Box Approach within the Isothermal-Isobaric Ensemble
- Xiaoyu Liang, Jeffrey Errington
- 9:00 Paper 659d: Free Energy Calculations Along Entropic Pathways: Application to Capillary Phase Transitions
- Caroline Desgranges, Jerome **Delhommelle**
- 9:15 Paper 659e: Determining the Predictability of Clusters Expansions By **Quantifying Their Associated Errors** - Greg Collinge, Alyssa Hensley, Jean-Sabin McEwen
- 9:30 Paper 659f: Development of Physics-Informed Neural Network Potentials for Molecular Simulations
- **Shih-Han Wang**, Hongliang Xin, Luke Achenie
- 9:45 Paper 174e: Molecular Dynamics Simulations to Study the Tribological Behavior of Gel-Forming Polymers for Cement-Based 3D Printing Applications
- Hajar Taheri Afarani, Babajide Y. Onanuga, Venkat Padmanabhan, Joseph J. Biernacki
- 10:00 Paper 659h: Nano-Thermodynamic Model Based on Distribution Coefficients for Understanding Segregation in Metal Alloy Nano Particles
- Gargi Agrahari, Abhijit Chatterjee
- 10:15 Paper 659i: Computing Solid-Liquid Interfacial Free-Energy Via Thermodynamic Integration
- Ravi Kumar Reddy, **Sudeep Punnathanam**

(660) Separation Processes in **Biorefineries**

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Discovery 47 Bandaru V. Ramarao, Chair Shri Ramaswamy, Co-Chair

Sponsored by: Forest and Plant **Bioproducts Division**

- 8:00 Paper 660a: An Electric Drive for Biorefineries: Electrochemical pH-Shift Liquid-Liquid Extraction of Succinic Acid
- Marcel Gausmann, Andreas Jupke
- 8:17 Paper 660b: Design and Optimization of an Acetic Acid Recovery System Via Extraction-Distillation Using an Isopropyl Acetate+Isopropanol Mixed Solvent
- Peng Fang, Li Sun, Zuoxiang Zeng, Weilan Xue

- 8:34 Paper 660c: Reactive Extraction of Acetic Acid from Liquid Phase Pyrolysis Oil and Solvent Regeneration By Distillation
- **Tanja Weiß**, Daniela Painer, Klara Treusch, Nikolaus Schwaiger, Peter Pucher, Matthaeus Siebenhofer
- 8:51 Paper 660d: Modulation of Lignin Inhibition on Lignocellulose Hydrolysis - Antonio C. F. dos Santos, Eduardo Ximenes, Nathan S. Mosier, Michael R.
- 9:08 Paper 660e: Modeling and Optimization of the Hydrolysis of Cellulosic Fibers by Integration of Membrane Separations and Enzyme Recycle - **Surya Jampana**, Bandaru V.
- 9:25 Paper 660f: Robust, High-Performance Graphene Oxide Nanofiltration and Reverse Osmosis Membranes for Black Liquor Concentration

Ramarao

Ramarao

- Sankar Nair, Zhongzhen Wang, Chen Ma, Scott Sinquefield, Meisha L.
- 9:42 Paper 660g: Optimization Study of Microalgae Dewatering By Utilizing Bio-Based Alkali
- Sheriff Ajala, Matthew L. Alexander
- 9:59 Paper 660h: Renewable Deep Eutectic Solvents (DES): Making Possible the Biochemical Conversion of Lignin
- Andrea Salgado, Angela Viteri, Carlos A. Alvarez-Vasco
- 10:16 Paper 660i: Purification of Lignocellulosic Hydrolyzate using Flocculant enhanced Depth Filters - Chenyi Lyu, Zewen Shen, Xuehao Wu, Thomas D. Stuart, Bandaru V.

(661) Sustainability and Consumer **Products**

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Regency Ballroom V William M. Barrett, Chair

Sponsored by: Sustainability Science and Engineering

- 8:00 Paper 661a: Synthesis and Performance Evaluation of New Bleach Activators
- Xue (Ida) Chen, Ziyuan Song, Jianjun Cheng, Steve King
- 8:25 Paper 661b: Sustainable Product Design: A Life-Cycle Approach — Xiang Zhang, Lei Zhang, Ka Y Fung, Bhavik R. Bakshi, Ka Ming Ng
- 8:50 Paper 661c: Combined Life Cycle Analysis and Environmental Risk Assessment As a Tool to Evaluate the Circular Economy of Plastics
- Rachael H. Rothman, Rukayya Ibrahim Muazu, Jonathan Howse, Lorraine Maltby

- 9:15 Paper 661d: Sustainability Potential of Melamine Non-Woven Prepared As a High-Performance Material for Thermal and Acoustic Applications
- Annamaria Vujanović, Lidija Čuček, Damjan Murn, Marjan Ješelnik, Christoph Kindler, Igor Mihelič, Simona Lavrič
- 9:40 Paper 661e: Shaping Technology Innovation: A Multistage, Multiscale Sustainability Assessment and Decision Support Framework
- Raha Gerami, Yinlun Huang

(662) Synthesis and Characterization of Materials for Optical and **Electronic Applications**

Thursday, Nov 14, 8:00 AM Hyatt Regency Orlando, Celebration 15 Joshua Choi, Chair Charles Hages, Co-Chair

Sponsored by: Electronics and

- 8:00 Paper 662a: Molecular **Engineering of Two-Dimensional** Organic-Inorganic Hybrid Perovskites - Letian Dou
- 8:20 Paper 662b: A General Deposition Method of and Optimization of Quantum-Cutting, Doped Metal-Halide Perovskite Films for Highly **Efficient Photovoltaics**
- Matthew Crane, Daniel M. Kroupa, Daniel Gamelin
- 8:40 Paper 662c: Spanning the Atomic to the Agglomerate Dimensions in Colloidal Dispersions of 2D Lead Halide Perovskites
- Clayton J. Dahlman, Naveen R. Venkatesan, Patrick T. Corona, Rhvs M. Kennard, Noah Smith, Matthew E. Helgeson, Michael L. Chabinyc
- 9:00 Paper 662d: Continuous on-Demand Synthesis of Perovskite Quantum Dots
- Milad Abolhasani
- 9:20 Paper 662e: Design of Semiconductor Surface Pits for Fabrication of Regular Arrays of **Quantum Dots and Nanorings** - Ashish Kumar**, Chao-Shou Chen**, Dimitrios Maroudas
- 9:40 Paper 662f: Synthesis of Metal Phosphide Nanocrystals for Optoelectronics
- Ingrid J. Paredes, Scott Lee, Mersal Khwaja, Rito Yanagi, Ayaskanta Sahu
- 10:00 Paper 662g: Molecularly Thin All-Solid-State Non-Volatile Memory Gated By a Monolayer Electrolyte - Jierui Liang, Ke Xu, Maokun Wu, Weihua Wang, Kyeongjae Cho, Susan Fullerton-Shirey

(663) Systems and Quantitative Biology: From Communities to Single Cells

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Celebration 4
Nathan Crook, Co-Chair
Chang Liu, Co-Chair
Laura Jarboe, Co-Chair

Sponsored by: Bioengineering

8:00 Paper 663a: Environmental Chemical Diethylhexyl Phthalate Alters Intestinal Microbiota Community Structure and Metabolite Profile in Mice — *Ming Lei, Kyongbum Lee*

8:18 Paper 663b: Increasing the Dimensionality of Single Cell Transcriptomics: Proteins, Imaging, and More

— Alex Xu, Qianhe Liu, Kaitlyn Takata, Sarah Jeoung, Yapeng Su, Sisi Chen, Igor Antoschechkin, Matthew Thomson, James R. Heath

8:36 Paper 663c: Cellular
Heteorgeneity in Endocytic Nanoarticle
Uptake: Dissecting the Origin Using
Quantitative Experiments and Modeling
— *Md Shahinuzzaman*, *Dipak Barua*

8:54 Paper 663d: Decoding Cross-Talk between HOG and Mating Pathways in Yeast through Mathematical Modeling and Single-Cell Analysis

— **Anik Chaturbedi**, Taylor Scott, Ping Xu, Megan McClean

9:12 Paper 663e: Quantitative Single-Cell Analysis of RNA Regulation at the Single-Molecule Level

— Fangyuan Ding, Michael Elowitz

9:30 Paper 663f: Metabolic Modeling of Cystic Fibrosis Airway Communities Predicts Mechanisms of Pathogen Dominance

— **Michael A. Henson**, Poonam Phalak, Giulia Orazi, George A. OToole

9:48 Paper **663g**: Synthetic Ecology for Bioproduction and Biosensing — *Cynthia Collins*

(664) Thermodynamics Needs of the Chemical Industry

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Silver Spring

J Richard Elliott, Chair Sumnesh Gupta, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

8:00 Paper 664a: Opening Comments for Session on Thermodynamics Needs of the Chemical Industry

- Sumnesh Gupta

Chris Muzny

8:20 Paper 664b: Current State of Thermophysical Property Measurements and Reporting in Scientific Publications — *Ala Bazyleva*, *Eugene Paulechka*, *Vladimir V. Diky, Joseph W. Magee*,

8:45 Paper 664c: An Improved Spectroscopic Method for Determination of Association/Solvation Parameters Used in Process Models

— William G. Killian, Aseel M. Bala, Lars Peereboom, Jackson A. Storer, Andrew T. Norfleet, James E. Jackson, Carl T. Lira

9:10 Paper 664d: A Molecular-Based Screening Tool for Water-Free Amine Solvents for CO₂ Capture

— **Ismail I. Alkhatib**, Luis M.C. Pereira, Ahmed Al Hajaj, Mohammad Abu Zahra, Lourdes F. Vega

9:35 Paper **664e**: Relationship of Solubility and Thermodynamic Parameters for Amine-Containing Non-Regenerative H₂S Scavengers

- Linh Doan, Tracy J. Benson

10:00 Paper 664f: Minimizing Process Development Costs in Industry By Computational Molecular Modeling Screening: Separation of Enantiomers for Pharmaceutical Applications

— **Xiaoyu Wang**, Cynthia J. Jameson, Sohail Murad

(665) Water Treatment, Desalination, and Reuse I

Thursday, Nov 14, 8:00 AM
Hyatt Regency Orlando, Barrel Spring I
Isabel Escobar, Co-Chair
William A. Phillip, Co-Chair
Mahdi Malmali, Co-Chair

Sponsored by: Membrane-Based Separations

8:00 Paper 665a: Centrifugal Reverse Osmosis (CRO) - a Novel Process for Achieving Desalination at the Thermodynamic Restriction

— **William B. Krantz**, Tzyy Haur Chong, Daniel J. Chen

8:21 Paper 665b: Functionalized Cellulose Nanocrystal Nanocomposite Membranes with Controlled Interfacial Transport for Improved Reverse Osmosis Performance

— **Ethan D. Smith**, Stephen M. Martin, Earl J. Foster, Keith Hendren, Jacob Haaa

8:42 Paper 665c: Systematic Evaluations of Pervaporation Performance and Property Calculations for Water Treatment

— **Elisabeth Thomas**, Mary Laura Lind, Kristina Luong

9:03 Paper 665d: Evaluating Pretreatment Technologies to Mitigate Fouling/Scaling in Membrane Distillation

— I-Min Hsieh, Mahdi Malmali

9:24 Paper 665e: Selective Separation of Industrial Relevant Metal Ions from High Tds Water Using Wafer-Enhanced Electrodeionization (WE-EDI)

— **Humeyra B. Ulusoy Erol**, Christa N. Hestekin, Jamie A. Hestekin 9:45 Paper 665f: Development of Robust, Ion-Selective Polymeric Ionic Liquid Composites for Reduced Energy Consumption within Water Purification Via Electrodialytic Separations

— Saloumeh Kolahchyan, Angela Fasuyi, **Alexander M. Lopez**

10:06 Paper 665g: Biomimetic, Nitrogen-Selective Adsorbents for Water Treatment and Fertilizer Production — *William A. Tarpeh*

(666) Ammonia Synthesis: Next Generation Technology III

Thursday, Nov 14, 10:20 AM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

10:20 Paper 666a: A Techno-Economic Model for Renewable Ammonia By Electrochemical Synthesis with Proton Conductive Membrane

— **Jamie Gomez**, John Baca, Fernando Garzon

10:43 Paper 666b: Ammonia Yields during Plasma-Assisted Catalysis Boosted By Hydrogen Sink Effect — *Maria Carreon*

11:06 Paper 666c: Synthesis and Assessment of Process Systems for Production of Ammonia Using Nitric Oxide in Combustion Exhaust Gas

— Hideyuki Matsumoto, Shotaro Ogawa, Keisuke Kobayashi, Tetsuya Nanba, Shiro Yoshikawa, Taku Tsujimura, Hirohide Furutani

11:29 Paper 666d: Mechanistic Insights into Electrochemical Nitrogen Reduction Reaction on Vanadium Nitride Nanoparticles

— **Xuan Yang**, Jared Nash, Shyam Kattel, Jingguang G. Chen, Yushan Yan, Bingjun Xu

11:52 Paper 666e: Ammonia Synthesis from Water and Nitrogen Under Ambient Condition Using Single Atom Nickel
— Shreya Mukherjee, Gang Wu

(667) Adsorbent Materials for Sustainable Energy and Chemicals

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Manatee Spring I

Marcus Mello, Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 667a: CO₂/H₂O Sorption Behaviour of Nickel Nanowires Immobilized in Silica Aerogels for the CO₂ Hydration Reaction

— **Vladimir Martis**, Khalil T. Hassan, Jiabin Wang Wang, Xiao Han, Lidija Siller

12:48 Paper 667b: Effects of Acid Gases in a Chemically Stable Metal-Organic Framework

— Eli A. Carter, Julian T. Hungerford, Jayraj Joshi, Xiao Jiang, Bartosz Marszalek, Ryan Lively, Krista S. Walton **1:06** Paper **667c:** Biomimetic, Molecularly-Designed Adsorbents for Selective Nitrogen Separations in Wastewater

— William A. Tarpeh

Siepmann, Laura Gagliardi

1:24 Paper **667d:** Metal-Catecholate Incorporated UiO Type MOFs for Natural Gas Upgrading and Toxic Gas Capture — *Hakan Demir, Samuel J.*Stoneburner, Christopher Cramer, J. Ilja

1:42 Paper 667e: Shape-Controlled Cuprous Chloride Crystals for Selective CO Adsorption

— **Farshad Feyzbar K Nejad**, Tae-Sik Oh

2:00 Paper 667f: Hydrogen Sulfide Removal from Biogas on Nitrogen-Doped Hierarchical Carbons

- Wenying Quan

2:18 Paper 667g: Selective Removal of Trace Propyne from Propylene Using Ion-Containing Materials

— **Tian Ke**, Jin Shen, Xin He, Qingju Wang, Zongbi Bao, Zhiguo Zhang, Huabin Xing, Qiwei Yang, Ren Qilong

2:36 Paper 667h: Trace Removal of CO₂ from LNG Using Advanced Materials — *Majeda Khraisheh*, *Jamileh Fouladi*, *Fares Almomani*

(668) Adsorbent Materials: MOFs

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Manatee Spring II Bin Mu, Chair

Sasidhar Gumma, Co-Chair

Sponsored by: Adsorption and Ion Exchange

12:30 Paper 668a: High-Throughput Screening of Metal-Organic Frameworks to Identify Best Materials for Biogas Upgrading

— **Hakan Demir**, Christopher Cramer, J. Ilja Siepmann

12:52 Paper 668b: Topological Effects on Separation of Alkane Isomers in Metal-Organic Frameworks

— N. Scott Bobbitt, Randall Q. Snurr

1:14 Paper 668c: Microporous MOFs with Specific Binding Sites for Trace Gas Contaminants Removal

— **Jun Wang**, Shuguang Deng

1:36 Paper 668d: Hierarchical MOF Nanoparticles for Natural Gas Liquids Adsorption

— Xinyang Yin**, Xueyi Zhang**

1:58 Paper 668e: Metal-Organic Frameworks As Food Spoilage Indicators

— Thomas Virdis, Joeri Denayer

2:20 Paper 668f: Gas Adsorption Properties of NH₂-MIL-53(Al) Metal Organic Framework: Experimental and Modeling Insights

— Mudit Baurai, Prudhviraj Medikonda, Prashant Mishra, Satyannarayana Edubilli**, Sasidhar Gumma** **2:42** Paper 668g: Ultrahigh CO₂/CH₄ and CO₂/N₂ Adsorption Selectivities on a Cost-Effectively L-Aspartic Acid Based Metal-Organic Framework

— Daofei Lv, Ying Wu, Jing Xiao, **Qibin** Xia, **Zhong Li**

(669) Advanced Biomass Conversion Technologies

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Discovery 47 Xinshu Zhuang, Chair Shijie Liu, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

12:30 Paper 669a: Subcritical CO₂-Assisted Autohydrolysis for the Co-Production of Oligosaccharides and Fermentable Sugar from Corn Straw — *Shubin Wu, Xiao Liu*

12:52 Paper 669b: Cell Wall Disruption in Low Temperature By KOH/Urea and Potential Application of Its Liquid Waste in Crop Production

— Xinshu Zhuang, Zahoor Zahoor, Wen Wang, Xuesong Tan, Qiang Yu, Zhenhong Yuan

1:14 Paper 669c: Lignocellulosic Biomass Derived N and S Doped Porous Carbon for Efficient Oxygen Reduction Reaction

— Xu Zhang

1:36 Paper 669d: Oxidation and Depolymerization of Alpha,Gamma-Diol-Protected Lignin into Aromatic Monomers

- Wu Lan, Jeremy S. Luterbacher

1:58 Paper 669e: Hybrid Dilute Sulfuric Acid and Aqueous Ammonia Pretreatment for Improving Butanol Production from Corn Stover with Reduced Wastewater Generation

— **Guangqing Du**, Chuang Xue

2:20 Paper 669f: Kinetic Study of Dissolution of Biochar in Tetralin — Rahul Kundu, Hema Ramsurn

2:42 Paper 669g: Techno-Economic Analysis of Production of Mixed-Furans from Biomass Hydrolysate

— **Ravikumar Gogar**, Sridhar Viamajala, Patricia Relue, Sasidhar Varanasi

(670) Advanced Treatment for Water: Advanced Oxidation Processes

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Rainbow Spring I/II Sage R. Hiibel, Chair M.Toufig Reza, Co-Chair

Sponsored by: Water

12:30 Paper 670a: Designing an Electrochemical System for Simultaneous Extraction of CO₂ and Rejection of Salts from Seawater — *Aditya Prajapati, Meenesh R. Singh*

12:45 Paper 670b: Breakdown Products from Perfluorinated Alkyl Substances (PFAS) Degradation in a Plasma-Based Water Treatment Process — Raj K. Singh, Sujan Fernando,

— Raj K. Singh, Sujan Fernando, Sadjad F. Baygi, Nicholas Multari, Thomas Holsen, **Selma Mededovic Thagard**

1:00 Paper 670c: Hydrothermal Degradation of Emerging Pollutants from Water

— **Nepu Saha**, M.Toufiq Reza

1:15 Paper 670d: Study the Degradation and Adsorption Processes of Organic Matters from Domestic Wastewater Using Chemically Prepared and Green Synthesized Nano Zero-Valent Iron

— Rabie Farag, Maha M. El-Shafei, Ahmed S. Mahmoud, Mohamed K. Mostafa, Ahmed Karam, **Robert W. Peters**

1:30 Paper 670e: Formic Acid Oxidation By the Fenton and Fentonlike Reaction: Experimental Study and Kinetic Modelling

— **Anke Arts**, Thijs de Groot, Riaan Schmuhl, John van der Schaaf

1:45 Paper 670f: Photolytic Inactivation of Cryptosporidium Parvum and Escherichia coli By Ultraviolet Radiation within a Microfluidic Reactor – Experimental and Modeling Development

— Christine Nguyen, **Omar Mohamed**, Matthew Coblyn, Goran Jovanovic, Tala Navab-Daneshmand

2:00 Paper 670g: Generation of Wastewater Treatment Networks: Integrating Process Efficiency, Economics and Sustainability

— Kirti M. Yenkie, Sean Burnham, Rohan Zia, Heriberto Cabezas

(671) Advances in Biocatalysis : Bioprospecting and Enzyme Engineering

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 1 Ryan M. Summers, Chair Joshua K. Michener, Co-Chair Nigel Reuel, Co-Chair

Sponsored by: Bioengineering

12:30 Paper 671a: Promiscuity of Dirigent Proteins and Their Application for Lignan Analog Synthesis

- Seung Yeon Kim, Elizabeth Sattely

12:48 Paper 671b: Prospecting
Thiamine Diphosphate-Dependent
Carboligases and Characterizing Their
Promiscuity to Create Novel Metabolic
Pathways from Primary Metabolites

— Bradley W. Bings. Jonathay Strutz

Pathways from Primary Metabolites
— Bradley W. Biggs, Jonathan Strutz,
Sara Wixon, Joseph Ni, Matthew
T. Robey, Valerie Winton, William
Corcoran, Paul M. Thomas, Neil L.
Kelleher, Linda J. Broadbelt, Keith E.J.
Tyo

1:06 Paper 671c: Discovery and Chararacterization of a Class IV Lanthipeptide with a Novel Ring Topology

— **Hengqian Ren**, Chengyou Shi, Wilfred A. van der Donk, Huimin Zhao

1:24 Paper 671d: Engineering of Oxidative Stress-Tolerant Yeast to Support Continuous Biomanufacturing of Chemicals from Acetate

- Wasti Nurani, Uffe H. Mortensen

1:42 Paper 671e: Directed Evolution of Oxygenases *In Vivo* Using a High-Throughput, Growth-Based Selection Platform

— **Sarah Maxel**, Linyue Zhang, Ana Paula Acosta, Derek Aspacio, Han Li

2:00 Paper 671f: De Novo Stereospecific Biosynthesis of 1,2-Propanediol

— **Wei Niu**, Levi Kramer, Joshua Mueller, Jiantao Guo

2:18 Paper 671g: Application-Driven Biocatalyst Discovery and Optimization — *Robert DiCosimo*

(672) Big-Data for Process Applications

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 26 Q. Peter He, Chair Fani Boukouvala, Co-Chair

Sponsored by: Data and Information Systems

12:30 Paper 672a: Sensor Fusion with Irregular Sampling and Varying Measurement Delays

— Joel Sansana, Ricardo Rendall, **Zhenyu Wang**, Leo H. Chiang, Marco Reis

12:49 Paper **672b**: Knowledge-Based Interactive Preprocessing of Process Data

— **Zhongyan Liu, Min Hong**, Min-Yi Peng, Yi Heng

1:08 Paper 672c: Data-Driven
Predictive Monitoring and Operation
Support for Change-over Processes
in Biopharmaceutical Drug Product
Manufacturing

— **Anicia Zeberli**, Sara Badr, Christian Siegmund, Markus Mattern, Hirokazu Sugiyama

1:27 Paper 672d: A Decision
Support Tool and Closed-Loop Startup
Framework for a Hydrogen Plant
— Abhinav Garg, Prashant Mhaskar,
Gangshi Hu, Jesus Flores-Cerrillo

1:46 Paper 672e: Using Channel State Information for Estimating Moisture Content in Wood Via 5 GHz Wi-Fi — Kerul Suthar, Forest Dewberry, Zhihua Jiang, Q. Peter He

2:05 Paper 672f: Identification of Repeating Sequential Alarms in Historical Operation Data of Chemical Plants

— **Ai Yanaga**, Masaru Noda

2:24 Paper 672g: Big Data for Enhanced Reduced Order Modeling: Application to Hydraulic Fracturing — Mohammed Saad Faizan Bangi, Abhinav Narasingam, Prashanth Siddhamshetty, Joseph Sang-Il Kwon

2:43 Paper 672h: A Clustering Decomposition Algorithm for Energy Storage Design & Operation — William W. Tso, C. Doga Demirhan, Clara F. Heuberger, Joseph B. Powell, Efstratios N. Pistikopoulos

(673) Bio-Based Polymers Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration

Shudipto Konika Dishari, Chair Danielle J. Mai, Co-Chair

Sponsored by: Polymers

12:30 Break

12:45 Paper 673b: Trimming Lignin Chemistry for Advanced Manufacturing of Renewable Carbon Fibers

— **Qiang Li**, Cheng Hu, Mengjie Li, Joshua Yuan

1:00 Paper 673j: Lignin based Ion Conducting Polymers with Controlled Ion Exchange Capacities (IECs) for Energy Conversion and Storage Devices
— Seefat Farzin, Shudipto Konika

1:15 Paper 673d: Isosorbide and Glucarodilactone-Based Polyethers and Poly(ester-thioethers) Via Ring-Opening and Photointiated Thiol-Ene Polymerization

— Theresa M. Reineke, Derek Saxon, Leon Lillie

1:45 Paper 673j: Tuning Rheological Behavior of Polymer-Nanoparticle Hydrogels for Injectable Drug Delivery — *Hector Lopez Hernandez*, *Anthony C. Yu, Eric A. Appel*

2:00 Paper 673f: Tetra-Functional Furan-Based Epoxy-Amine Thermosetting Systems with Superior Characteristics

— **Xi Chu**, Jian Gao, John La Scala, Giuseppe Palmese

2:15 Paper 673g: Investigations into the Fabrication of Chitin Nanofibers Using Supercritical Anti-Solvent Precipitation

— Amy L. Lindenberger, Sunggyu Lee

2:30 Paper 673h: Synergistic Interactions of Chitin Nanofibers and Cellulose Nanocrystals in Blended Films with Enhanced Barrier Properties

— Chinmay C. Satam, Cameron W.

— Chinmay C. Satam, Cameron W. Irvin, Cameron J. Coffey, Riley K. Geran, Meisha L. Shofner, J. Carson Meredith

2:45 Paper **673i**: Coarse-Grained Simulations of Grafted Methylcellulose Chains — *Vaidyanathan Sethuraman*, *Kevin D. Dorfman*

(674) Biomaterials

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 10 Kelly A. Burke, Chair Wei Li, Co-Chair Jorge Almodovar, Co-Chair Piyush Jain, Co-Chair

Sponsored by: Biomaterials

- 12:30 Paper 674a: Dynamic Covalent Hydrogels As Responsive Biomaterials — Bruno Marco-Dufort, Mark W. **Tibbitt**
- 12:48 Paper 674b: Integration of Electrodes into Polymer Scaffolds for Near-Uniform Electric Field Distribution during Irreversible Electroporation
- Francisco Pelaez, Pegah Ranjbartehrani, Qi Shao, Tiffany Lam, Hak Rae Lee, Stephen O'Flanagan, Abby Silbaugh, John C. Bischof, Samira M. Azarin
- 1:06 Paper 674c: Heparin-Collagen Layer-By-Layer Coatings Enhance Adhesion and Proliferation of Schwann Cells for Nerve Tissue Regeneration - Luis Carlos Pinzon-Herrera, Jorge Almodovar
- 1:24 Paper 674d: Engineering Tunable Growth Factor Release Rates and Degradation Rates from Silk-Extracellular Matrix Scaffolds
- Julie F. Jameson, Jonathan M. Grasman, Elizabeth C. Bender, Alexa M. Espinoza, Lauren D. Black III, David L. Kaplan, Whitney L. Stoppel
- 1:42 Paper 674e: Straining Red Blood Cells with Liquid Crystals
- Karthik Nayani, Saverio Spagnolie, Nicholas L. Abbott
- 2:00 Paper 674f: Influence of Composition on of Physiochemical Properties of Lactic Acid and Sebacic **Acid Copolymers**
- Eswar Arunkumar Kalaga, Timothy M Brenza
- 2:18 Paper 674g: Using Rheology to Quantify the Effects of Injectable Collagenase Treatments on Strength and Viscoelasticity of Mammalian Tissues - Ria D. Corder, Saad A. Khan
- 2:36 Paper 674h: Bio-Adhesion Properties of the Attachment Cement from the Tick Species Dermacentor Marainatus
- Laura L. E. Mears, Laila Moreno Ostertag, Christian Cupak, Johannes Suppan, Marian Fürsatz, Benedikt Engel, Martina Marchetti-Deschmann, Orestis Andriotis, Philipp J Thurner, Sylvia Nürnberger, Markus Valtiner

(675) Biomaterials for Drug Delivery: **Particles & Colloids**

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 14 **Matthew Webber, Chair** Mathumai Kanapathipillai, Co-Chair Sutapa Barua, Co-Chair

Sponsored by: Biomaterials

- 12:30 Paper 675a: Multi-Drug Loaded **BIOMOFs Clear Mycobacterium Tuberculosis Infection**
- **Abhinav P. Acharya**, Kutay Berk Sezginel, Ashlee Greene, Nathaniel L. Rosi, Christopher E. Wilmer, Steven Little
- 12:48 Paper 675b: Self-Assembling Protides Nanofibers and Their Application to Anticancer Drug Delivery - Carston R. Wagner, Harrison T. West, Nicole Bentz
- 1:06 Paper 675c: Galactosylated **Dendrimer Targets Hepatocytes and** Improves Therapeutic Outcomes in a Severe Model of Acetaminophen Poisoning
- Joshua E. Porterfield, Rishi Sharma, Aniali Sharma, Ambar Jimenez, Sam Norwood, Sujatha Kannan, Rangaramanujam Kannan
- 1:24 Paper 675d: Nanoparticle Hitchhiked T Cells for Targeted Drug Delivery
- Muhammad Raisul Abedin, Yongjian Liu, Sutapa Barua
- 1:42 Paper 675e: Controlled Microfluidic Synthesis of Polymeric Nanoparticles for Drug Delivery
- Giovanni Bovone, Mark W. Tibbitt
- 2:00 Paper 675f: Designing Ionic Solvents for Transdermal Delivery
- Eden E L Tanner, Samir Mitragotri
- 2:18 Paper 675g: Stimuli-Responsive Hydrogel Microparticle Populations As a 'Plug and Play' Model for Creating Controlled and Tailorable Therapeutic Delivery
- Paige LeValley, April M. Kloxin
- 2:36 Paper 675h: Hydrophobized Nanogels for the Delivery of Poorly Water Soluble Therapeutics to the Brain
- **Madeline Simpson**, Ugonwa Echendu, Ali Babar, Ram K. Mishra, Todd R. Hoare

(676) Bionanotechnology for Gene and Drug Delivery II

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Discovery 45 Joo-Youp Lee, Chair Piyush Jain, Co-Chair

Sponsored by: Bionanotechnology

- 12:30 Paper 676a: Effect of Laser Irradiation on Drug Release and Nano-Structural Reversibility of Light-Activatable Methotrexate-Encapsulated Liposomes
- Saikat Das, Robert Lazenby, Yuan Zheng, Ryan White, Yoonjee Park
- 12:48 Paper 676b: Near Infrared, One-Photon Triggered Liposome Cage for Calcium, ATP or Both
- JeongEun Shin, Anisha Veeren, Maria Olu Ogunyankin, Joesph A. Zasadzinski
- 1:06 Paper 676c: Cholesterol Content Mediates Tumor Cell Uptake of Targeted Linosomes
- **Stephanie M. Kong**, Paula T. Hammond

- 1:24 Paper 676d: Serum Effects on Nanoparticle-Mediated Photoporation for Enhanced Intracellular Drug Delivery — Simple Kumar, Eunice Lazau,
- Carter Kim, Cameron Chong, Naresh N. Thadhani, Mark R. Prausnitz
- 1:42 Paper 676e: Autophagy Targeting Nano-Prodrugs for Synergistic Therapy of Metastatic Cancer
- Wang Huifang, Liu Xiangrui, Shen
- 2:00 Paper 676f: ROS-Responsive Doxorubicin Prodrug for Effective Breast **Cancer Treatment**
- Vishnu Sriram, Mina Jafari, Joo-Youp Lee
- 2:18 Paper 676g: Engineering pH Responsive, Self-Assembled Polymer Nanoparticles for the Oral Delivery of **Protein Therapeutics**
- Matthew Miller, Michael Elder, Lexi Lakatta, Nicholas A. Peppas
- 2:36 Paper 676h: Systemic Dendrimer-Mediated Delivery of Triptolide Specifically to Tumor-Associated Macrophages Improves Efficacy in Glioblastoma
- Kevin Liaw, Rishi Sharma, Sujatha Kannan, Rangaramanujam Kannan

(677) Case Studies in Technology: Design, Risk Reduction and Implementation

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 18 John Peragine, Chair Raymond E. Rooks, Co-Chair

Sponsored by: Technology Transfer and Manufacturing

- 12:30 Paper 677a: Rapid Risk Assessment and Process Optimization to Enable FIH
- Adam Freitag, Jason Zhu, James Paulson, Benjamin M. Cohen, Michael Schmidt, Qinggang Wang, Amanda Rogers
- 12:52 Paper 677b: Optimizing Continuous Twin-Screw Wet Granulation for a Batch to Continuous Conversion Qiushi Zhou, Fernando J. Muzzio
- 1:14 Paper 677c: Regeneration Scaleup Methodology Applied to Bio-Based Isobutanol Dehydration to Linear **Butenes**
- Nicolas Aribert. Adrien Mekki-Berrada, Vincent Coupard, Nikolai Nesterenko, Colin Dupont, Kirill Drobvshev
- 1:36 Paper 677d: Design and Implementation of Robust Multicomponent Working Fluid for Organic Rankine Cycle
- Kyeongsu Kim, Jeongnam Kim, Ung Lee
- 1:58 Paper 677e: Study on Ozone Formation Characterization during the Flaring of Chemical Plant Shutdown for Proactive Flare Minimization and Air-**Quality Control**
- Sijie Ge, Sujing Wang, Qiang Xu, Thomas Ho

- 2:20 Paper 677f: CFD-FEA Analysis for Scale-up of a Twin Screw Extruder **Kneading Block Section**
- Laura J. Dietsche, Gulab Malunikar, Joseph Jacobs, Anthony Neubauer
- 2:42 Paper 677g: Investigation of Soil Corrosive Effect on Buried Gas Pipeline: **New Correlation Development** Bizhan Honarvar

(678) Catalysis for Biomass **Upgrading II: Novel Catalytic Materials**

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Florida Ballroom B

Juan J. Bravo-Suarez, Chair Kenneth L. Roberts, Co-Chair

Sponsored by: Catalysis and Reaction **Engineering Division**

- 12:30 Paper 678a: Understanding Diffusion and Catalyst Deactivation in the Chemical Funneling of Lignin Derived Monomers over Zeolites
- Michael Stellato, Marina Pinho Oncken, Matthew Realff, Andreas S. Bommarius, Carsten Sievers
- 12:48 Paper 678b: Tuning the Paraffinto-Olefin Ratio in High-Octane Gasoline Synthesis Using Bimetallic BEA Zeolite Catalysts
- Daniel P. Dupuis, Connor P. Nash, Anh T. To, Carrie A. Farberow, Susan Habas, Jesse E. Hensley, Daniel A. Ruddy
- 1:06 Paper 678c: Evaluating Zeolite Supported Pt/ZIF-67 with Low Noble-Metal Loading for the Deoxygenation of Saturated and Unsaturated Fatty Acids — James M. Crawford, Moises A.
- 1:24 Paper 678d: Phosphorus-Substituted Zirconium Metal-Organic Frameworks with Bronsted Acidity and Their Versatility for Biomass Catalysis Matheus Dorneles de Mello. Gaurav Kumar, Paul Dauenhauer, Michael Tsapatsis
- 1:42 Paper 678e: Cooperative Co (0)/ Co (II) Sites Stabilized By a Perovskite Matrix Enable Selective C-O and C-C Bond Hydrogenolysis of Oxygenated Arenes
- Manish Shetty, Daniela Zanchet, William H. Green, Yuriy Román-Leshkov
- 2:00 Paper 678f: Upgrading Glycerol Via Selective Hydrodeoxygenation Reaction on Copper-Modified Molybdenum Carbide and Nitride Surfaces
- Zhexi Lin, Steven R. Denny, Weiming Wan, Salai C. Ammal, Kyung-Eun You, Andreas Heyden, Jingguang G. Chen
- 2:18 Paper 678q: Investigating the Role of Oxophilic Modifiers in Bimetallic Catalysts for Enhanced Hydrodeoxygenation
- Mathew Rasmussen, J. Will Medlin

- 2:36 Paper 678h: Enhanced Aromatic Selectivity during Deoxygenation of Phenolic Model Compounds over Bifunctional Catalysts
- **Yang Xiao**, Anand Ramanathan, Bala Subramaniam, Arvind Varma

(679) Catalytic Hydrocarbon Processing II: Ethane, Propane, and Light Hydrocarbons

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom E William W. Lonergan, Chair Yizhi Xiang, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 679a:** Structure Sensitivity of n-CnH_{2n-2} hydrogenolysis on Supported ir Catalysts
- **Xiwen Zhang**, Yubing Lu, Prasanna Dasari, Dick Nagaki, Ayman M. Karim
- 12:50 Paper 679b: Oxidative Dehydrogenation of Propane on Boron Nitride Catalyst: A Computational Investigation of Active Site As Well As Involved Mechanism Using Boron Nitride Nanoribbons
- Andreas Heyden, Biplab Rajbanshi
- **1:10** Paper 679c: Formation of Proton-Hydride Pair and Its Kinetic Significance for Heteroarene Hydrogenation in Hydrotreating and Hydrodeoxygenation Reactions
- Haiting Cai, Manos Mavrikakis, Haoyu Nie**, Ya-Huei (Cathy) Chin**, Roberto Schimmenti
- **1:30** Paper 679d: *In Situ* Spectroscopic Analysis of Reactive Hydrocarbon Surface Species and Their Transformations *Eric D. Hernandez, Friederike C.*
- Jentoft, Babgen Manookian, Scott M. Auerbach
- **1:50** Break
- **2:10** Paper 679f: Catalytic Ethane Conversion through Ammoxidation *Xia Liu, Tingyu Liang, Yizhi Xiang*
- 2:30 Paper 679g: Monodisperse Au-FeCx Bimetallic Catalysts for Selective Synthesis of Higher Alcohols from Syngas — Zhuang Zeng, Yue Wang, Xinbin Ma

(680) Characterization and Measurement in Powder Processing Thursday, Nov 14, 12:30 PM

Hyatt Regency Orlando, Bayhill 21 Pavithra Sundararajan, Chair Michael Winn, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- **12:30 Paper 680a:** A Course at Purdue University on Particle, Powder, and Compact Characterization
- **Kingsly Ambrose**, Dhananjay A. Pai, Carl Wassgren
- **12:48** Paper 680b: Non-Linear Dependence of Macroscopic Powder Properties on Powder Composition *Sara Fathollahi*, Eva Faulhammer, Benjamin Glasser, Johannes G. Khinast

- **1:06** Paper **680c:** Comparative Study of Sugar Powder Consistency Using an FT₄ Powder Rheometer and Drag Force Flow (DFF) Sensor
- **John Yin**, Valery Sheverev, Vadim Stapaniuk
- **1:24** Paper 680d: Material Property Database and Its Applications in Predictive Batch and Continuous Unit Operation Modeling
- **Pallavi Pawar**, Antonio Benedetti, Jingzhe Li, Don Clancy, Fernando J. Muzzio, Robert E. Yule
- **1:42 Paper 680e:** Wide Range Particle Sizing for Submicron By Scattering Light Image Analysis
- **Tomonari Misawa**, Jun Tanaka, Yoshiki Yonamoto
- **2:00** Paper **680f**: Polymer and Metalic Powders Flowability & Electrical Charges Characterisation for Additive Manufacturing
- Filip Francqui, Geoffroy Lumay
- **2:18 Paper 680g:** Characterizing the Effect of Powder Flow Aid Additives
- **Geoffroy Lumay**, Filip Francqui
- **2:36** Paper 680h: On the Feasibility of Utilising Compaction Equation Parameters As Material Key Attribute Descriptors
- **Samuel Solomon**, Ahmad B. Albadarin

(681) Computational Approaches to Protein Engineering

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 3 Yongku Cho, Chair Jerome M. Fox, Co-Chair Bradley C. Bundy, Co-Chair

Sponsored by: Bioengineering

- **12:30 Paper 681a:** A Novel Interaction-Oriented Approach for Predicting Off-Target Antibody Specificities
- Varun Chauhan, Robert Pantazes
- **12:48 Paper 681b:** Developing Similarity Matrices for Protein-Protein Interactions
- **Sumaiya Islam**, Robert Pantazes
- 1:06 Paper 681c: Quantitative Characterization of Protein-Ligand and Protein-Protein Binding Processes Involved in Plant Hormone Signaling
- **Chuankai Zhao**, Jiming Chen, Faisal Aldukhi, Alexander Moffett, Diwakar Shukla
- **1:24 Paper 681d:** Poredesigner: A Computational Tool for the Design of Membrane Pores for Separations
- Ratul Chowdhury, Costas Maranas
- **1:42** Paper **681e**: Computational Protein Design Targeting Oxidized RNA Modifications
- **Asuka A. Orr**, Juan Camilo Gonzalez, Sean M. Engels, Joseph M. Jakubowski, Brendan C. Woodcock, Lydia M. Contreras, Phanourios Tamamis

- 2:00 Paper 681f: Paired Simulations and Experimental Investigations into the Calcium-Dependent Bioactivity of Albumin
- **Dharmeshkumar Patel**, Jagdish Suresh Patel, Stephanie Haag, F. Marty Ytreberg, **Matthew T Bernards**
- 2:18 Paper 681g: Designing Protein Structures and Complexes with the Molecular Modeling Program Rosetta — Brian Kuhlman

(682) Deoxygenation and Oxidation in Biomass Upgrading

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom F Ning Yan, Chair Peng Bai, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- 12:30 Paper 682a: Solvent System for Effective Production of Hydroxymethylfurfural (HMF) with Potential for Process Integration into Current High Fructose Corn Syrup (HFCS) Infrastructure
- **Ali Hussain Motagamwala**, Kefeng Huang, Christos T. Maravelias, James A. Dumesic
- **12:48** Paper 682b: Hydrogen Rich Syngas Production through Synergistic Methane Activated Catalytic Biomass Gasification
- **Amoolya Lalsare**, Yuxin Wang, Qingyuan Li, Ali Sivri, Roman Vukmanovich, Cosmin Dumitrescu, Jianli Hu
- **1:06** Paper **682c:** Selective Hydrodeoxygenation of Guaiacol to Phenolics By Anatase TiO₂ supported Ni Atoms
- **Z. Conrad Zhang**, Xiaoqiang Zhang, Peifang Yan, Kairui Liu, Mayfair Kung, Harold H. Kung
- 1:24 Paper 682d: Deactivation Pathways of Raw Bio-Oil Hydrodeoxygenation over Noble Metal Supported Bifunctional Catalysts
- Tomás Cordero-Lanzac, Roberto Palos, Idoia Hita, José Rodríguez-Mirasol, Tomás Cordero, Javier Bilbao, Pedro Castaño
- **1:42** Break
- 2:00 Paper 682f: Aqueous Oxidation of Xylose to Xylonic Acid over Synergistic PtCu Catalysts Using Molecular O₂
- **Jie Ding**. Hao Yan, Mengyuan Liu, Jingyao Wang, Qi Xia, Xin Jin
- 2:18 Paper 682g: High Yield of Succinic Acid Production through Deoxydehydration/Hydrodeoxygenation Reactions of Tartaric Acid
- **Ayad Nacy**, Génesis Ruiz-Valentín, Gerardo Rivera-Castro, Sandra Albarracín-Suazo, Yomaira J. Pagan-Torres

- 2:36 Paper 682h: Rhenium Catalyzed Conversion of Sugar Acids to Adipates Via Deoxydehydration and Hydrogen Transfer Using Isopropyl Alcohol

 Jun Hee Jang, Mahdi Abu-Omar
- (683) Development of Pharmaceutical Process Control Strategies for Production of Biologics Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 6 Samrat Mukherjee, Chair Daniel L. Obrzut, Co-Chair
- **Sponsored by:** Pharmaceutical Discovery, Development and Manufacturing Forum
- **12:30 Paper 683a:** Constrained Optimisation of Cell Culture Feeding Strategy and Temperature Shift Duration to Enhance Monoclonal Antibody Titre and Purity
- **Sakhr Alhuthali**, Sarah Fadda, Cleo Kontoraydi
- 12:55 Paper 683b: Control of Glycosylation and Titer in Fed-Batch Monoclonal Antibody Production — Yu Luo, Devesh Radhakrishnan, Anne Robinson, Babatunde A. Ogunnaike
- 1:20 Paper 683c: Using High-Throughput Microbioreactors to Fit Raman Spectroscopy Model for Measuring Key Metabolites in Monoclonal Antibody Cell Culture Manufacturing Process
- Michael Nelson, Marek Hoehse, Christian Grimm, Angus Woodhams, Mark Brower, Douglas Richardson, Matthew Manahan, Ikechukwu Nwaneshiudu, Jack Huang
- 1:45 Paper 683d: Evaluation of Process Parameters Influencing Immobilized Metal Affinity Chromatography — Robert Clifford, Ellen O'Connor, Christopher L. Thompson, Valeria Riguero
- **2:10 Paper 683e:** Investigation of Bio-Capacitance Driven Process Variation in a Site to Site Large Scale Technology Transfer Campaign
- Haofan Peng**, Patrick Johnstone**, Erik Hughes
- 2:35 Paper 683f: Characterization of Rotary Lobe Pump Damage in Large-Scale Cell Culture Perfusion Process — Patrick Johnstone, Haofan Peng, Erik Hughes

(684) Developments in Alternative Fuels and Enabling Technologies I

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Challenger 38/39

Helen H. Lou, Chair Gaurav Agrawal, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

- **12:30 Paper 684a:** Development of a Hydrogen Impurity Enrichment Device Using Pd Alloy Membranes to Support the Growing Hydrogen Economy
- Marc Plunkett, K. Li, Arul Murugan

- 12:55 Paper 684b: Shock Tube Study of Co-Optima Biofuels Combustion
 Erik Ninnemann, Andrew Laich, Sneha Neupane, Samuel Barak, Subith Vasu
- 1:20 Paper 684c: Production and Characterization of Biorenewable Thermal Deoxygenation Oil/ Ultra Low-Sulfur Diesel Blends
- **Sampath A. Karunarathne**, Scott J. Eaton, Matthew J. Kline, M. Clayton Wheeler
- 1:45 Paper 684d: Acid-Catalyzed Rearrangement of Tetrahydrotricyclopentadiene: Synthesis of High-Density Alkyl-Diamondoid Fuel — Jiawei Xie, Li Wang, Xiangwen Zhang, Lun Pan, Ji-Jun Zou
- 2:10 Paper 684e: Advanced Gamma-Ray Densitometry (GRD) Technique to Measure Gas and Liquid Holdups in Bench Scale Hydrotreater Reactors — Mohammed Al-ani, Muthanna Al
- 2:35 Paper 684f: Extraction of Essentials from Petroleum Sludge: A Review

 Utkarsh Maheshwari, Amit
 Chimurkar

(685) Drug Delivery II Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 2 Srivatsan Kidambi, Chair

Srivatsan Kidambi, Chair Greg Thurber, Co-Chair Jessica Larsen, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

12:30 Break

Dahhan

- **12:48 Paper 685b:** Carrageenan/ Starch (SeaGel®) Films As Gelatin Alternative for Soft-Shell Capsule Applications
- **Jin Zhao**, Benjamin Roscoe, Andrew Horton, Harold Bernthal
- **1:06 Paper 685c:** Electrospun Transdermal Patch for Contraceptive Hormone Delivery
- **Mohammad Mofidfar**, Mark R. Prausnitz
- **1:24 Paper 685d:** Personalising Dosage Forms By 3D Printing and Computer Simulation
- **Matej Novak**, Pavel Kovačík, Zdenek Grof, Tereza Boleslavska, František Štěpánek
- 1:42 Paper 685e: Dispersion of Drug Particles and Emulsion Drops in Oleogels for Ophthalmic Drug Delivery — Russell Macoon
- **2:00 Paper 685f:** Mechanism of Transdermal Delivery of Macromolecules Assisted By Ionic Liquids
- Qin M. Qi, Samir Mitragotri
- 2:18 Paper 685g: Contact Lens Based Drug Delivery to the Posterior Segment Via Iontophoresis in Cadaver Rabbit Eyes
- Keith Christopher, Anuj Chauhan

- **2:36 Paper 685h:** Microneedles for Cutaneous Peanut Allergen Immunotherapy
- **Harvinder Singh Gill**, Akhilesh Shakya, Chang Hyun Lee

(686) Electrochemical CO₂ Reduction I: Fuels

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom D Feng Jiao, Chair Carlos Morales Guio, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 686a:** Electrolyte Based Tuning of CO₂ Electroreduction Selectivity on Copper Surfaces
- **Sneha A. Akhade**, Stephen E. Weitzner, Felicia R. Lucci, Jeremy T. Feaster, Joel B. Varley, Brandon C. Wood, Sarah E. Baker, Eric B. Duoss
- **12:48** Paper **686b**: Copper Oxide Quantum Dots for Electrochemical Reduction of Carbon Dioxide to Methane
- Mohammadreza Esmaeilirad, Alireza Kondori, Andres Ruiz Belmonte, Shubhada Mahesh Khanvilkar, Erin Efimoff, Mohammad Asadi
- **1:06 Paper 686c:** Steering Selectivity in CO₂ Electrocatalysis Towards Value-Added Fuels and Chemicals
- Thomas F. Jaramillo
- **1:24** Paper **686d:** Binding Site Diversity Promotes CO_2 Electroreduction to Ethanol
- **Yuguang (Chris) Li**, Ziyun Wang, Edward Sargent
- 1:42 Paper 686e: Demonstration of One-Pot Tandem Catalysis for Electrochemical CO₂ Reduction to CH₄ Using Both Quantum Mechanics and Experiment
- **Haochen Zhang**, Mu-Jeng Cheng, Qi Lu
- **2:00 Paper 686f:** Multimetallic Core-Shell Nanoporous Pd Alloys for Surface Poisoning Suppression during Electrohydrogenation of CO₂ to Formate
- **Swarnendu Chatterjee**, Charles Griego, Yawei Li, John A. Keith, Joshua Snyder
- **2:18** Paper 686g: The Chemisorption Scaling of CO₂R Intermediates on Carbon Nanotube Surfaces with High-Curvature
- **Michael Tang**, Karen Chan, Jens K. Norskov
- **2:36 Paper 686h:** Leveraging Advanced Manufactured Catalysts and Reactors for Electrochemical CO₂ Conversion
- **Jeremy T. Feaster**, Felicia R. Lucci, Zhen Qi, Marissa Wood, Joshua R. Deotte, Nikola Dudukovic, Siwei Liang, Clara L. Druzgalski, Victor Beck, Wenqin Li, Sarah Baker, Eric B. Duoss

(687) Energy Sustainability: Challenges and Solutions

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Regency Ballroom U Emre Gençer, Chair Vikas Khanna, Co-Chair

William M. Barrett, Co-Chair

Sponsored by: Sustainability Science and Engineering

- **12:30 Paper 687a:** A Process Systems Integration Tool to Build Energy Efficiencies in Biorefineries: Selection of Processes to Save Energy and Boost Cogeneration
- **Konstantinos A. Pyrgakis**, Antonis C. Kokossis
- **12:55** Paper **687b**: Geospatial Assessment of Waste Heat from Unconventional Oil and Gas Production *Elmira Mohammadi Shamlou*.

Radisav Vidic, Vikas Khanna

- 1:20 Paper 687c: Novel Approach for Weighting in Geographic Information System Focused on a Multi-Stakeholder Problem: Case for Residual Biomass Processing System
- José Ezequiel Santibañez Aguilar, Diego Fabián Lozano-García, Antonio Flores-Tlacuahuac, Francisco José Lozano
- **1:45 Paper 687d:** Liquid Organic Hydrogen Carrier and Their Application at Moderate Temperatures
- Karsten Müller
- **2:10 Paper 687e:** Production of (Bio) Butanol By Means of a Design for Sustainability Methodology
- Jessica Sanchez-Ramirez, David Vargas-Lopez, Lilia Arteaga-Espinoza, **Edgar Ramirez-Jimenez**

(688) Fluidization and Fluid-Particle Systems for Energy and Environmental Applications

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 19 Fangxing Li, Chair Jing Huang, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

- **12:30** Paper **688a**: The Effect of Ambient Gas Species on Tribocharging *Xiaoyu Liu, Jari Kolehmainen, Ah-Hyung Alissa Park, Sankaran Sundaresan*
- **12:51 Paper 688b:** CFD-PBM Simulation of Catalytic Coal Hydrogasification in a Pressurized Fluidized Bed
- **Zihong Xia**, Shuai Yan, Caixia Chen, Jicheng Bi, Xuan Qu
- 1:12 Paper 688c: DDPM-DEM
 Simulation of Biomass Gasification in a
 Bubbling Fluidized Bed Reactor
 In Sik Hwang, Jungho Hwang

- 1:33 Paper 688d: Kinetic Modeling of Low-Temperature PM Combustion with Relative Velocity in the Presence of Water Vapor
- **Kento Yokoo**, Tsuyoshi Yamamoto, Hideki Matsune, Masahiro Kishida, June Tatebayashi
- **1:54** Paper **688e**: Particle Attrition By Chemical Reaction during the Redox Process of Chemical Looping Combustion
- Nathan Galinsky, **Samuel Bayham**, Ronald W. Breault
- 2:15 Paper 688f: Intensification of Ethylene Production By Chemical Looping Oxidative Dehydrogenation through Exergy Loss Minimization Luke Neal, Vasudev Pralhad Haribal, Fanxing Li
- 2:36 Paper 688g: Synthesis and Characterization of Aerosol Particles and Reactions for the Solar Driven Hybrid-Sulfur-Ammonia Water-Splitting Cycle
 Navaira Fathima, Agni E. Kalyva, Athanasios G. Konstandopoulos, Rahul Bhosale, Konstantinos E. Kakosimos

(689) Fundamentals of Surface Chemistry I

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Florida Ballroom A

John R. Di Iorio, Chair Daniel T. Bregante, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **12:30 Paper 689a:** Relating Local Coordination to Function for Oxide Supported Pt Atoms
- **Joaquin Resasco**, Phillip Christopher
- **12:48** Paper 689b: Characterization of Surface Species during Benzene Hydroxylation over a NiO on Ceria-Zirconia Catalyst
- **Jennifer Jocz**, Yimeng Lyu, Carsten Sievers
- **1:06** Paper 689c: Active Site Dynamics in Atomically Dispersed Catalysts

 Shaama Mallikarjun Sharada
- **1:24** Paper **689d:** Atomically Dispersed Rh-Lewis Acid Sites Pairs for Selective Methanol Carbonylation to Acetic Acid *Ji Qi, Phillip Christopher*
- 1:42 Paper 689e: Predicting the Surface Phase Diagram of Ag(111) Using Ab Initio Grand Canonical Monte Carlo — Robert B. Wexler, Tian Qiu, Andrew M. Rappe
- 2:00 Paper 689f: Spectro-Kinetic Observations of Ligand Exchanges for Single-Site Supported Metal Catalysts through the Development of QXAS at
- Adam Hoffman, Oliver Mueller, Chia-Yu Fang, Jorge Perez-Aguilar, Bruce Gates, Simon R. Bare

- 2:18 Paper 689g: On the Bottomup Design of Bimetallic Catalytic Nanoparticles with Atomic Level Resolution
- **Tej S. Choksi**, Verena Streibel, Luke Roling, Frank Abild-Pedersen
- **2:36 Paper 689h:** Computational Design of Sub-Surface Engineered Metal Oxides for Catalysis
- Liang Zhang

(690) Gas Hydrates Science and Engineering

Thursday, Nov 14, 12:30 PMHyatt Regency Orlando, Peacock
Spring

Praveen Linga, Chair Amadeu Sum, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **12:30** Paper **690a**: Kinetic Hydrate Inhibitors: Gas Hydrate Induction Time Probability Distributions and Deviations from Classical Nucleation Theory
- Vincent W.S. Lim, Peter J. Metaxas, Paul L. Stanwix, Michael L. Johns, Zachary M. Aman, Eric F. May
- **12:47 Paper 690c:** Structure H Hydrate Formation with Lmgs and CO₂, in Ice and Water
- **Namrata Gaikwad**, Omkar Singh Kushwaha, Praveen Linga, Jitendra Sangwai, Rajnish Kumar
- 1:04 Paper 690d: Understanding the Influence of Thermodynamic Hydrate Inhibitors on the Mechanics of Cyclopentane Hydrate Films Using Interfacial Rheology with Subphase Exchange
- David M. Goggin, **Joseph R. Samaniuk**
- 1:21 Paper 690e: Insight into the Hydrate Nucleation of Structure II Propane Hydrates from Molecular Simulation
- Amadeu Sum, Yong Chen
- 1:38 Paper 690f: Modeling the Effects of Interfaces on the Nucleation of Gas Hydrates and Ice in Porous Media
- Yali Zhang, **Patricia Taboada**-**Serrano**
- 1:55 Paper 690g: A Fundamental Comparison of the Stability and Dissociation Aspects of Structure I and Structure II Hydrates from the Perspective of Feasible Natural Gas Storage
- **Gaurav Bhattacharjee**, Hari Prakash Veluswamy, Rajnish Kumar, Praveen Linga
- **2:12 Paper 690h:** Container-Free Gas Hydrate Nucleation Using High-Pressure Acoustic Levitation
- **Kwanghee Jeong**, Peter J. Metaxas, Zachary M. Aman, Paul L. Stanwix, Michael L. Johns, Eric F. May

(691) Going to a Decision Point in Sustainability Analysis

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Blue Spring I/II Madhav Ghanta, Chair Ángel Galán Martín, Co-Chair

Sponsored by: Sustainability

- **12:30** Paper **691a:** Estimating True Cost of Ionic Liquids Using Monetization
- **Husain A. Baaqel**, Ismael Diaz, Jason P. Hallett, Benoit Chachuat, Gonzalo Guillén-Gosálbez
- **12:55** Paper **691b**: Optimised Actions to Engage Cooperative Partnerships for an Effective Climate Change Mitigation
- Ángel Galán Martín, Carlos Pozo Fernández, Adisa Azapagic, Ignacio E. Grossmann, Niall Mac Dowell, Gonzalo Guillén-Gosálbez
- 1:20 Paper 691c: Achieving Campus Carbon Neutrality - Application of Sustainable Engineering Methods to Evaluate and Identify Technical and Ecological Solutions
- Michael Charles, Bhavik R. Bakshi
- 1:45 Paper 691d: Attributional to Consequential Life Cycle Assessment – Steps Toward a Unified Framework
- **Tapajyoti Ghosh**, Kyuha Lee, Bhavik R. Bakshi
- **2:10 Paper 691e:** Noise Abatement That Substantiated to be Fiscal for Ammonia Complex
- **Sara Ahsan**, Arsalan Naeem

(692) Inhomogeneous Polymers Thursday, Nov 14, 12:30 PM

Hyatt Regency Orlando, Celebration 5

Jeffrey M. Ting, Chair
Iman Noshadi, Co-Chair

Sponsored by: Polymers

- **12:30** Paper **692a**: Heteropolymer Design and Synthesis through Practical Prediction of Controlled Radical Polymerizations
- Anton A. A. Smith, Aaron Hall, Vincent Wu, Eric A. Appel, Ting Xu
- **1:00** Paper 692b: Design of Sustainable Graft Block Polymer Plastics *Alice B. Chang, Frank S. Bates*
- **1:15 Paper 692c:** Theory of Sequence-Controlled Complex Coacervation
- **Artem Rumyantsev**, Boyuan Yu, Nicholas Jackson, Juan de Pablo
- 1:30 Paper 692d: Impact of Nanoparticle Dispersion and Surface Chemistry on the Segmental Dynamics and Transport Properties of Ionomer Nanocomposites
- **Apoorv Balwani**, Allison Domhoff, Antonio Faraone, Eric M. Davis
- 1:45 Paper 692e: Design of Block Copolymers to Form Chiral Mesophases (single gyroid) Using Particle-Based Simulations
- Natalie Buchanan, Krysia Browka, Hillary Le**, Poornima Padmanabhan**

- 2:00 Paper 692f: In-Silico Dynamic Properties of the "Bricks-and-Mortar" Mesophase from Binary Miktoarm Star Block Copolymer/Homopolymer Blends — Cody Bezik, Abelardo Ramirez-Hernandez, Juan J. de Pablo
- **2:15 Paper 692g:** Simulating Diblock Copolymer Micelles in Binary Explicit Solvents
- **Dong Meng**, Jing Zong
- 2:30 Paper 692h: Towards 3D Nanopatterning in Polymeric Gels Using Photochromic Switches
- **Harikrishnan Vijayamohanan**, Edmund Palermo, Chaitanya Ullal
- **2:45** Paper **692i**: Chromogenic Photonic Crystal Sensors for Detecting Molecular Diffusion in Polymers
- **Calen Leverant**, Sin-Yen Leo, Peng Jiang

(693) Innovations and Emerging Technologies: Automated Platforms and Novel Methodologies

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 7 Nigel Reuel, Chair David J. am Ende, Co-Chair

Sponsored by: Pharmaceutical Discovery, Development and Manufacturing Forum

- **12:30** Paper **693a**: Data-Rich Development of a Novel Biocatalytic Aerobic Oxidation across Scales
- **Shane T. Grosser**, Sandra A. Robaire, Jacob H. Forstater, Ania Fryszkowska, Keith A. Mattern, Christopher C. Nawrat
- **12:51** Paper **693b**: Automated Platform for Experimental Execution and Model Regression of Volumetric Mass Transfer Coefficient and Vessel Characterization *Keith A. Mattern, Shane T. Grosser*
- **1:12** Break
- 1:33 Paper 693d: Continuous Manufacturing of Oral Disintegrating Films: Impact of Manufacturing Process Parameters on Product Quality
- **Sonal Mazumder**, Scott M. Krull, Nima Yazdanpanah, Xiaoming Xu, Muhammad Ashraf, Celia N. Cruz, Thomas O'Connor, Naresh Pavurala
- **1:54** Paper **693e**: The Development of a Predictive Tableting Platform in the Context of Continuous Direct Compression
- Thomas De Beer
- **2:15 Paper 693f:** Drug Form Considerations in Continuous Solution Processing of Oral Solid Dosage Products
- Elena Ewaldz, **Blair Kathryn Brettmann**
- 2:36 Paper 693g: Half Tablet Methodology: Investigating the Relationship between Dissolution Behavior and Raman Change Inaging
- **Shashwat Gupta**, Andres Roman, Doug Hausner, Fernando J. Muzzio

(694) Ionic Liquids: Novel Separation and Reaction Processes

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Regency Ballroom Q

Kevin N. West, Chair Suojiang Zhang, Co-Chair Dickson E. Ozokwelu, Co-Chair Brooks D. Rabideau, Co-Chair Xiangping Zhang, Co-Chair

Sponsored by: Innovations of Green Process Engineering for Sustainable Energy and Environment

- **12:30 Paper 694a:** Discovery of New Ionic Liquids Via Molecular Simulations for the Separation of Azeotropic Mixtures of High Global Warming Potential Hydrofluorocarbon Refrigerants
- **Bridgette Befort**, Alexander W. Dowling, Edward Maginn
- **12:48 Paper 694b:** Commercial Applications of Ionic Liquids
- Mark B. Shiflett
- 1:06 Paper 694c: Whole-Cell Bioconversion of Phytosterols in Ionic Liquids Co-Solvents with Alleviation of Product Inhibition
- **Xia Xiao**, Yi-Xin Guan, Shan-Jing Yao
- **1:24** Paper 694d: Study of [Rmim] [Al₂Cl₇] Using a Low AlCl₃/[Rmim]Cl Molar Ratio As Electrolytes in Aluminum Electrolysis at 60 oc
- **Junshi Wu**, Wenbin Hao, Yongli Mi
- 1:42 Paper 694e: New Application of Ionic Liquids As a Sweep Fluid in Methanol Synthesis in a Membrane Reactor
- **Fatemeh Sadat Zebarjad**, Sheng Hu, Theodore Tsotsis
- **2:00** Paper 694f: Sulfuric Acid-Catalyzed Isobutane Alkylation with C₄ Olefin Promoted By Sulfonic-Acid-Functionalized Ionic Liquids
- **Weizhen Sun**, Piao Cao, Ling Zhao
- 2:18 Paper 694g: Composite Adsorbents with Anion-Pillared Microporous Materials Embedded in Poly (Ionic Liquids) for Flue Gas Desulfurization
- **Siheng Qian**, Xili Cui, Ling Xia, Xian Suo, Huabin Xing
- 2:36 Paper 694h: The Catalytic
 Mechanisms and Performances of Ionic
 Liquids in Green Reaction Processes

 Xiaoqian Yao

(695) Life Cycle Analysis of Bio-Based Fuels, Energy, and Chemicals Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Regency

Ballroom T
David R. Shonnard, Chair
Yuan Yao, Co-Chair
Eric Tan, Co-Chair

Sponsored by: Sustainable Biorefineries

- **12:30 Paper 695a:** Modeling the Impact of Solar Tracking on Life Cycle Greenhouse Gas Emissions from Photovoltaic Power
- **Emre Gençer**, Ian Miller, Sarah Torkamani, Francis O'Sullivan
- **12:55 Paper 695b:** Life Cycle Carbon Footprint of Renewable Electricity Generation from Aspen Forest Harvest in Wisconsin, USA
- Olumide Winjobi, Ulises R. Gracida-Alvarez, Michelle Cisz, Rod Chimner, Sigrid Resh, **David Shonnard**
- 1:20 Paper 695c: Miscanthus
 Sacchariflorus Bioenergy Production
 Peter Zhao, Benjamin J. Davis, Dave
 Chun, Amanda Simson
- 1:45 Paper 695d: Evaluating Variability of Energy Consumption and Carbon Emissions of Activated Carbon Production from Wood Using Artificial Neural Network Integrated Process Simulation Mochen Liao, Steve Kelley, Yuan Yao
- 2:10 Paper 695e: Understanding the Uncertainties in Environmental Life Cycle Energy and Carbon Analysis for Biofuel from Forest Residue in the United States
- Kai Lan, Longwen Ou, Stephen S. Kelley, Sunkyu Park, Hoyoung Kwon, Hao Cai, Michael Wang, Yuan Yao
- 2:35 Paper 695f: Well-to-Wake
 Analysis of Switchgrass to Butanol Via
 Co-Fermentation of Sugar and Gas with
 Subsequent Conversion to Jet Fuel
 Abhiram Pamula, David J. Lampert,
 Hasan K. Atiyeh

(696) Lithium and Beyond: Fundamental Advances in High Performance Batteries II

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Plaza International Ballroom I Robert J. Messinger, Chair Lauren Marbella, Co-Chair

Sponsored by: Electrochemical Fundamentals

- **12:30 Paper 696a:** Scalable Synthesis of Li₂S Nanocrystals for Use in Next Generation Batteries
- William Smith, Yangzhi Zhao, Colin A. Wolden
- **12:45** Paper 696b: Mitigation of the Polysulfide Shuttle Effect through Use of Crosslinked Ionomer Coatings
- Hunter Ford, Peng He, **Jennifer Schaefer**
- **1:00 Paper 696c:** Highly Energy Dense Cu-Intercalated Birnessite/Zn Battery for Grid Applications
- **Gautam G. Yadav**, Damon Turney, Jinchao Huang, Xia Wei
- 1:15 Paper 696d: Zinc Anode
 Discharge Study in Alkaline Electrolyte
 for Rechargeable Battery Applications
 Michael D'Ambrose, Damon Turney,
 Gautam G. Yadav, Michael Nyce, Sanjoy
 Baneriee

- **1:30 Paper 696e:** Tracking Percolation Pathways in Hybrid Solid Electrolytes for All Solid State Batteries
- **Kelsey Hatzell**, Marm Dixit, Wahid Zaman
- 1:45 Paper 696f: Evolution of Cathodic Interfaces with the Solid Electrolyte Li,La,Zr,O,
- **Alexander Delluva**, Jessica Dudoff, Adam Holewinski
- **2:00 Paper 696g:** Solubility of the Solid Electrolyte Interphase Layer Components
- **Ethan P. Kamphaus**, Perla B. Balbuena
- **2:15** Paper 696h: Molecular Structure and Dynamics of Lithium Polysulfide Clusters in Organic Solvent Mixture
- **Vijayakumar Murugesan**, Amity Andersen, Nav Nidhi Rajput, Kee Sung Han, Niranjan Govind, Karl Mueller
- 2:30 Paper 696i: Novel Cathode Framework of Nanostructured Titanium Nitride/Graphene for Advanced Lithium Sulfur Batteries
- **Wenduo Zeng**, Mark Cheng, Simon Ng
- **2:45** Paper 696j: A First-Principle Study on the Structure and Properties of Na-Se Alloys for Sodium Ion Battery
- Eunsu Paek

(697) Mixed-Matrix Materials for Gas Separation

Thursday, Nov 14, 12:30 PM
Hyatt Regency Orlando, Coral Spring I/II
Zachary P. Smith, Co-Chair
Michele Galizia, Co-Chair
Bin Mu, Co-Chair

Sponsored by: Membrane-Based Separations

- **12:30 Paper 697a:** Custom Formulation of Ultra-High Permeability Mixed-Matrix Membranes for Post-Combustion Carbon Capture
- **Sameh Elsaidi**, Surendar Venna, Mona Mohamed, Ali Sekizkardes, David Hopkinson
- **12:51** Paper **697b:** Highly Propylene-Selective Mixed-Matrix Membranes By *in-Situ* MOF Formation Using a Polymer-Modification Strategy
- Sunghwan Park, Hae-Kwon Jeong
- **1:12** Paper 697c: Natural Gas Sweetening By MOF-Polymer Hybrid Membranes with Tailored Formulation
- **Yang LIU**, William Koros, Zhijie Chen, Gongping Liu, Youssef Belmabkhout, Mohamed Eddaoudi
- 1:33 Paper 697d: Enhanced Gas Separation Performance and Plasticization Resistance through Mixed Matrix Membrane Approach Incorporating Multi-Dimensional Metal-Organic Frameworks
- **Won Seok Chi**, Benjamin J. Sundell, Ke Zhang, Daniel J. Harrigan, Steven C. Hayden, Zachary P. Smith

- **1:54 Paper 697e:** Ultra-Permeable Mixed Matrix Membranes Containing ZIF Nanoparticles for CO₂ Capture
- Leiqing Hu, Haiqing Lin, Jun Cheng
- **2:15 Paper 697f:** Adsorptive and Destructive Mixed Matrix Membranes for Chemical Protection
- Yufeng Song, **Kamalesh K. Sirkar**, Gregory W. Peterson, Uwe Beuscher
- **2:36** Paper **697g:** Ultrathin MOF-Based Mixed Matrix Hollow Fiber Membranes for Highly Efficient Carbon Capture
- **Shouliang Yi**, Patrick Muldoon, Ali Sekizkardes, Fangming Xiang, Victor A. Kusuma, Lingxiang Zhu, Nathaniel L. Rosi, Kevin P. Resnik, David Hopkinson

(698) Modeling of Interfacial Systems

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Orlando Ballroom N

Manuela A.A. Ayee, Chair David C. Cantu, Co-Chair

Sponsored by: Interfacial Phenomena

- **12:30 Paper 698a:** A Computational Study on Adsorption of Trialkoxysilane Functionalized Perfluoropolyether on Silica Surfaces
- **Yong Nam Ahn**, Sung Hoon Lee, Sangyoon Oh
- **12:44** Paper 698b: Modeling of Interfacial Properties and Interfacial Mass Transfer in Liquid-Liquid Extraction Systems
- **Roland Nagl**, Patrick Zimmermann, Tim Zeiner
- **12:58** Paper **698c:** Mechanism of Adsorption of Non-Ionic Surfactants on Calcite
- **Soumik Das**, Fardin Khabaz, Quoc P. Nguyen, Roger T. Bonnecaze
- 1:12 Paper 698d: Prediction of Surface Tensions and Adsorption Isotherms of Alkane Isomers
- Patrick Zimmermann
- **1:26** Paper 698e: Molecular Simulation on the Antifouling Mechanism of Zwitterionic Materials
- **Yiqi Chen**, Andrew J. Schultz, Jeffrey Errington
- 1:40 Paper 698f: First-Principles
 Design of Nerve Agent Sensing Systems
 Using Chemoresponsive Liquid Crystals
 Jake Gold, Tibor Szilvási, Nicholas L.
 Abbott, Manos Mavrikakis
- 1:54 Paper 698g: Examination of the Relationships between Terminal Group Chemistry and Tribological Properties in Monolayer Films through Molecular Dynamics Screening
- Christopher R. lacovella, Andrew Z. Summers, Justin Gilmer, Peter T. Cummings, Clare McCabe
- 2:08 Paper 698h: Simulations of the Diffusive Behavior of DNA Adsorbed on Charged Lipid Bilayers
- **I-an Chiang**, Chang Ming-Yi, Chih-Chen Hsieh

- **2:22 Paper 698i:** Predicting Contact Angle in Oil/Brine/Calcite Systems Using Molecular Simulations
- Mohamed S. AlHosani, **Arjun Valiya Parambathu**, Fernando Yrazu, Dilip Asthagiri, Walter G. Chapman
- 2:36 Paper 698j: Heat Transfer across Tip-Surface Nanointerface: A Quantitative Model By Scanning Thermal Microscopy (SThM)
- Yifan Li, Nitin Mehra, Jiahua Zhu
- 2:50 Paper 698k: Controlling Protein Crystallization through Wetting Near a Critical Point
- Jens Glaser, Sharon C. Glotzer

(699) Modular Processes for Coal and/or Biomass Conversion Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Challenger 41/42

David Lyons, Chair Jonathan W. Lekse, Co-Chair

Sponsored by: Advances in Fossil Energy R&D

- **12:30 Paper 699a:** Developing Low-Cost, Efficient, Gasification-Based Modular Energy Systems *David Lyons*
- **12:48** Paper 699b: Microchannel Based Distillation Technologies to Accomplish Process Intensification in Coal/Biomass Conversion
- Ward E. Tegrotenhuis
- 1:06 Paper 699c: Upgrading Coal for the Production of Value-Added Chemicals and Feedstocks By Wave Liquefaction": Spectroscopic Diagnostics and Material Characterization
- Akshay Gharpure, Raju Kumal, Randy Vander Wal, Kurt Zeller, George Skontsov
- **1:24** Paper **699d:** Analysis of the Heat Transfer in a Packed Bed Composed of Alumina and Coal Exposed to a High Thermal Radiation Flux
- **Mario G. Toledo Torres**, Nicolás A. Ripoll Kameid, Gustavo Ruiz Núñez
- 1:42 Paper 699e: Conversion of Coal Wastes and Municipal Solids Mixtures By Pyrolysis Torrefaction and Entrained Flow Gasification
- **Nicholas R. Schwartz**, Michael J. Blaise, Paul E. Yelvington
- 2:00 Paper 699f: Moving Bed Chemical Looping Reactor Systems for Power Generation and Hydrogen – Pilot Scale Testing and Process Analysis — Andrew Tong, Liang-Shih Fan
- 2:18 Paper 699g: Subcritical and Supercritical Water Gasification of Soybean Straw and Flax Straw for Hydrogen Production: Experimental and Thermodynamic Modeling
- **Ajay K. Dalai**, Jude A. Okolie, Sonil Nanda, Janusz A. Kozinski
- **2:36 Paper 699h:** A Compact System for Mass Production of Hydrogen from Biogas
- Chan Hyun Lee

(700) Nanomaterials for Biological Applications II

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Discovery 44 Cerasela Zoica Dinu, Chair Jaeyun Kim, Co-Chair

Sponsored by: Bionanotechnology

- 12:30 Paper 700a: Solid-Phase Synthesis of Megamolecules: A New Class of Nanoscale Therapeutics - Blaise Kimmel, Kevin Metcalf, Milan
- 12:45 Paper 700b: Developing Nanofiber-Based, Safe and Functional Cell Delivery Devices for Type 1 Diabetes — Minglin Ma
- 1:30 Paper 700c: Green Synthesis of a Synergetic Structure of Tellurium Nanowires and Metallic Nanoparticles for Biomedical Applications
- Ada Vernet Crua, David Medina, Jorae Luis Cholula Diaz, Jose Miauel Garcia Martin, Thomas J. Webster
- 1:50 Paper 700d: Graphene-Silk Fibroin and Noble Metal Nanocomposites for Biosensing Applications
- R. Kenneth Sims, Jenny Wang, Kenneth Brinson, Thomas Alvermann, Alexander Mitropoulos, Kamil Woronowicz, Pamela L. Sheehan, Preston Haney, Harry L. Moore, F. John Burpo, Enoch A. Nagelli
- 2:10 Paper 700e: Formulation of Super Paramagnetic Iron Oxide Nanoparticles for Cryoprotecting Agent Solutions - Andreina Chiu-Lam, Edward Staples, Carl Pepine, Carlos Rinaldi
- **2:25 Paper 700f:** Utilizing UiO-66 Metal-Organic Frameworks (MOFs) As Pulmonary Drug Delivery Vehicles
- Bader M. Jarai, Zachary S. Stillman, Gerald E. Decker, Lucas Attia, Shuja Abbas, Eric D. Bloch, Catherine A.
- 2:40 Paper 700g: Modeling Diblock-Arm Star Polymers for Drug Delivery **Applications**
- Kevin R. Hinkle

(701) Natural and Bio-Composites Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 11 **Zhe Wang, Chair** Asem Abdulahad, Co-Chair

Sponsored by: Composites

- 12:30 Paper 701a: Thermal Insulation Material Based on Poly Lactic Acid (PLA) and Date Palm Wood Powder (DPWP)
- Mohamed Barkhed. Basim Abu-Jdayil, Abdel-Hamid Mourad
- 12:55 Paper 701c: Thermal Conductivity Characteristics Based on Epoxy Resin and Pineapple Leaf Fiber - **Jyoti Jain**, Shishir Sinha, Shorab Jain

- 1:20 Paper 701d: Flame Retardant Characteristics of Natural Fiber and Bio Based Composites: Effect of Surface Treatments
- Jyoti Jain, Shishir Sinha, Shorab
- 1:45 Paper 701e: Relating Mechanical Properties of Biofilm-Mineral Composites to Bulk Consolidated Media **Properties**
- Sobia Anjum

(702) New Frontiers of Molecular Thermodynamics (Invited Talks)

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Silver Spring I/II Rajesh Khare, Chair Shekhar Garde, Co-Chair

Sponsored by: Thermodynamics and **Transport Properties**

- 12:30 Paper 702a: Molecular Design of Polymer Nanocomposites
- Robert A. Riggleman
- 1:00 Paper 702b: Coarse-Grained Models for Predicting Structure and Thermodynamics in Macromolecular Systems with Specific and Directional Intermolecular Interactions
- Arthi Jayaraman, Arjita Kulshreshtha
- 1:30 Paper 702c: Computational Design of Water-Mediated Interactions M. Scott Shell
- 2:00 Paper 702d: Characterizing Protein Hydration to Inform Its Interactions
- Nicholas Rego, Erte Xi, Amish J.
- 2:30 Paper 702e: Deep Learning of Slow Collective Variables to Understand and Accelerate Biomolecular Folding and Assembly
- Hythem Sidky, Wei Chen, Andrew **Ferguson**

(703) Particle Technology in Product Design

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 20 **Brenda Remy, Chair** Sebastian Escotet-Espinoza, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- 12:30 Paper 703a: Evaluating Different Dry Coating Processes for Preparing Fine-Grade High Functional Microcrystalline Cellulose
- Liang Chen, Sangah Kim, Kuriakose Kunnath, Kai Zheng, Rajesh Davé
- 12:48 Paper 703b: Characterization and Mitigation of Stick-Slip in Pharmaceutical Powders
- Marissa Amichetti, Christina Pothier, Rohit Kumar, Subhash Thakur, Shrikant Swaminathan
- 1:06 Paper 703c: Effect of Particle Properties and Formulation Composition on Sticking Behavior during Pharmaceutical Tabletting - Maxx Capece, Daniel Young

- 1:24 Paper 703d: Impact of Particles Needle Shape, a Critical Material Attributes (CMAs), on Miniaturized Pharmaceutical Units Operation
- **Mohammad Azad**, Gerard Capellades, Allison Wang, David Klee, Gregory Hammersmith, Kersten Rapp, David Brancazio, Allan Myerson
- 1:42 Paper 703e: Coarsening Approach in Modeling Gas-Particle Flows in Dry Powder Inhaler
- Xiaoyu Liu, Jari Kolehmainen, Sankaran Sundaresan
- 2:00 Paper 703f: Surface Engineering of Inhaled Pharmaceutical Particles By Atomic and Molecular Layer Deposition
- Damiano La Zara, Feilona Sun. Fuweng Zhang, Di Zhang, Mike J. Quayle, Gunilla Petersson, Staffan Folestad, J. Ruud van Ommen
- 2:18 Paper 703g: Magnetically Assisted Impaction Coating (MAIC) for Optimising Blending in Pharmaceutical Applications
- Tim Freeman, Katrina Brockbank, William A. Hendrickson, Charles R. Bowman, Christopher J. Rueb
- 2:36 Paper 703h: Linking Moisture Induced Variations in Pharmaceutical Primary Powders to Their Tableting Performance
- Rachael Shinebaum, Ian Gabbott, Gavin K. Reynolds, Hannah K. Batchelor, Andrew Ingram

(704) Practical Applications of **Computational Chemistry and Molecular Simulation II**

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Rock Spring I/II Phillip R. Westmoreland, Chair Jonathan Moore, Co-Chair

Sponsored by: Computational Molecular Science and Engineering

- 12:30 Paper 704a: A Deep Neural Network Model for MD-Level Packing Density Predictions and Its Application in the Study of 1.5 Million Organic Molecules — Johannes Hachmann
- 12:45 Paper 704b: Toward Better Solar Cells: First Principles Understanding of the Water Instability of Hybrid Perovskites
- Arvin Kakekhani, Andrew M. Rappe
- 1:00 Paper 704c: Simulation of the Surface Tension of a Nematic Liquid Crystal in Contact with a Planar Solid - Paul Brumby, Rik Wensink, Andrew J. Haslam, George Jackson
- 1:15 Paper 704d: Multi-Scale Simulation of Ionic Polyimide Composite Membranes Based on Structural and **Electrostatic Maps**
- C. Heath Turner, Henry Atkinson, Jason E. Bara

- 1:30 Paper 704e: Computational Design of Physical Solvents for Gas Separation
- Wei Shi, Jeffery Culp, Robert L. Thompson, Surya Tiwari, Kevin P. Resnik, Nicholas Siefert, Janice A. Steckel, David Hopkinson
- 1:45 Paper 704f: First-Principles Computational Study of the Adsorption Mechanism for CH₂I(g) Removal - **Hoje Chun**, Byungchan Han
- 2:00 Paper 704g: Binding Mechanism of Titania Binding Peptide (TBP) on Titania from MD Simulations
- Janani Sampath, Jim Pfaendtner
- 2:15 Paper 704h: Rapid Prediction of Adsorption in Hyper-Crosslinked Polymers: Expanding the Chemical Space for Adsorption and Separation Dai Tang, Grit Kupgan, Coray M. Colina, David S. Sholl
- 2:30 Paper 704i: Effects of Topology and Pore Size of Metal-Organic Frameworks on Their Adsorption and Transport Properties: Insights from Molecular Simulations
- Haoyuan Chen, Randall Q. Snurr
- 2:45 Paper 704j: Molecular Dynamic Simulation of Protein Devices: Pegylated Proteins and Protein Microarrays - Addison K. Smith. Joshua W. Wilkerson, Thomas A. Knotts IV

(705) Predictive Control and Optimization

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 25 Ali Mesbah, Chair Fernando V. Lima, Co-Chair

Sponsored by: Systems and Process Control

- 12:30 Paper 705a: On the Use of Recurrent Neural Network Models in **Economic Model Predictive Control of** Nonlinear Processes
- Zhe Wu, Scarlett Chen, David Rincon, Panagiotis D. Christofides
- 12:49 Paper 705b: Closed-Loop Dynamic Real Time Optimization with a Stable MPC Formulation
- Praveen Sundaresan Ramesh, Prashant Mhaskar, Christopher L. E.
- 1:08 Paper 705c: Robust Nonlinear Model Predictive Control with Scenario Reduction
- Zhou (Joyce) Yu, Lorenz T. Biegler
- 1:27 Paper 705d: Overlapping Domain Decomposition Schemes for Graph-Structured Optimization Problems
- Sungho Shin, Mihai Anitescu, Victor M. Zavala
- 1:46 Paper 705e: Autonomous Design of Advanced Control Systems for Modular Chemical Systems
- Matthias von Andrian, Anastasia Nikolakopoulou, Richard D. Braatz

- 2:05 Paper 705f: Fast Advanced-Step Economic MPC Based on Turnpike **Properties**
- Dinesh Krishnamoorthy, Lorenz T. Biegler, Johannes Jäschke
- 2:24 Paper 705g: A Multiparametric Programming-Based Approach for Multi-Objective Model Predictive Control
- **losif S. Pappas**, Styliani Avraamidou, Nikolaos A. Diangelakis, Efstratios N. Pistikopoulos
- 2:43 Paper 705h: Economic Linear Optimal Control with Model Uncertainty Jin Zhang, Donald J. Chmielewski

(706) Process Design: Innovation for Sustainability

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Regency Ballroom V

Dharik Mallapragada, Chair Aydin Sunol, Co-Chair

Sponsored by: Sustainability Science and Engineering

- 12:30 Paper 706a: Sustainable Dmc Production from CO₂ and Renewable Ammonia and Methanol
- Antonio Sánchez, Luis M. Gil, Mariano Martín
- 12:55 Paper 706b: Opportunity Cost-**Based Systematic Process Intensification Under Multiple Objectives**
- Akhilesh Gandhi, Salih E. Demirel, Jianping Li, M. M. Faruque Hasan
- 1:20 Paper 706c: Dynamic Optimization to Leverage Flexible Heat Integration within a Hybrid CSP Plant - Kevin Ellingwood, Kody M. Powell
- 1:45 Paper 706e: Thermodynamic Assessment of Innovative Routes for Acrylic Acid Production from Carbon Dioxide
- Jonas Laedson Marinho da Silva Santos, Alessandra de Carvalho Reis, Antonio Esio Bresciani, Rita M. B. Alves
- 2:10 Paper 706d: Designing Climate-Resilient Chemical Processes and Supply Chains
- Kyuha Lee, Sami Khanal, Bhavik R Bakshi
- 2:35 Paper 706f: Quantification of Physical and Monetary Benefits of Forest Ecosystem: A Case Study for Net Positive Impact Manufacturing - Utkarsh Shah, Bhavik R. Bakshi

(707) Process Intensification through the Application of Microreactors, **Multiphase Reactors, and Membrane** Reactors

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 17 Matthaus Siebenhofer, Chair Patrick Heider, Co-Chair Jing Luo, Co-Chair

Sponsored by: Process Intensification & Microprocess Engineering

12:30 Paper 707a: Process Intensification of the Alkoxylation of Fatty Amines - Pia Müller, Wyatt Winkenwerder, John van der Schaaf

- 12:52 Paper 707b: Process Intensification of Propane Dehydrogenation Using Microporous Silica Membranes
- Shailesh Dangwal, Anil Ronte, Seok-
- 1:14 Paper 707c: Scalable Thin-Layer Membrane Reactor for Heterogeneous and Homogeneous Catalytic Gas-Liquid Reactions
- Yiming Mo, Joseph Imbrogno, Haomiao Zhang, Klavs F. Jensen
- 1:36 Paper 707d: Plug Flow Membrane Reactor for Esterification of Acetic Acid with Mor-Type Zeolite Membrane
- Masahiko Matsukata, **Motomu** Sakai, Yuki Nonaka
- 1:58 Paper 707e: Advance Electrochemical CO₂ Utilization Towards Higher Industrial Readiness: Across Multiple Scales from Catalyst Design, Electrode Decoration, to Reactor Engineering
- Xu Lu
- 2:20 Paper 707f: Continuous-Flow Synthesis of the Azo Pigment Yellow 14 Using a Three-Stream Feeding Micromixer
- **Fajun Wang**, Jianhong Xu
- 2:42 Paper 707g: Enhanced Hydroformylation Reactions in Continuous Flow Honeycomb Fractal Microreactor
- Sijing Wang, Zhiyong Tang, Fei Peng, **Jie Zhang**, Yuhan Sun

(708) Supply Chain Management and Schedulina

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 24 Fengqi You, Chair Zuwei Liao, Co-Chair

Sponsored by: Computers in **Operations and Information Processing**

- 12:30 Paper 708a: Single Pad Planning Under Uncertainty for Shale Gas Development
- Can Li, Ignacio E. Grossmann, John P. Eason, Markus G. Drouven
- 12:49 Paper 708b: Multi-Mode Resource Constrained Project Scheduling for Pharmaceutical R&D
- Hua Wang, Shekhar Viswanath, Steve Guntz, Jon Dieringer, Shankarraman Vaidyaraman, Salvador García-Muñoz, Chrysanthos E. Gounaris
- 1:08 Paper 708c: Novel Discrete-Time MILP Scheduling Model for Pipeline Systems
- Hossein Mostafaei, liro Harjunkoski, Pedro M. Castro
- 1:27 Paper 708d: Optimal Scheduling of Parallel Distillation Column System with Continuous-Time Formulation
- Fanglin Shao, Xiang Li, Lingyu Zhu, Han Gong, Xi Chen
- 1:46 Paper 708e: Systematic Methods for Generating Multiple Alternative Schedules
- **Hojae Lee**, Dhruv Gupta, Christos T. Maravelias

- 2:05 Paper 708f: Simultaneous Scheduling for Refinery Plant Manufacturing and Downstream Multi-**Product Pipeline Distribution**
- Li Yu, Qiang Xu
- 2:24 Paper 708g: Combining Data Analytics and Scheduling – First Results and Open Challenges
- liro Harjunkoski, Teemu Ikonen, Hossein Mostafaei
- 2:43 Paper 708h: Improved Batch-Centric Formulation for Multiproduct Pipeline Scheduling
- Qi Liao, Pedro M. Castro, Yongtu Liang, Haoran Zhang

(709) Surface Engineered and **Responsive Membranes**

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Barrel Spring II Ayse Asatekin, Co-Chair Dona Foster, Co-Chair Ranil Wickramasinghe, Co-Chair

Sponsored by: Membrane-Based Separations

- 12:30 Paper 709a: Fouling-Resistant Block Copolymer Membranes By Simultaneous Selective Swelling and Zwitterization
- Chenxu Zhang, Jiemei Zhou**, Yong**
- 12:51 Paper 709b: Membranes with Non-Stick Surface to Mitigate Fouling for Water Purification
- Thien Tran, Yi-Chen Tu, Christopher M. Stafford, Haiging Lin
- 1:12 Paper 709c: Surface Modification of PVDF Membranes for Treating Produced Waters By Direct Contact Membrane Distillation
- Arijit Sengupta, S. Ranil Wickramasinghe
- **1:33** Break
- 1:54 Paper 709e: High-Performance Thin Film Composite (TFC) Membranes: Design Consideration Underneath the Polyamide Thin Film
- Wangxi Fang
- 2:15 Paper 709f: Crosslinked Mixed Matrix Polyimide Membranes Surface-Modified By Amine Vapor for Organic Solvent Nanofiltration
- **Zhuo Fan Gao**, Yingnan Feng, Dangchen Ma, Neal Tai-Shung Chung
- 2:36 Paper 709q: Ultrathin MOF/ Zeolite Membrane with Enhanced Separation Performance
- Zhi Xu

(710) Systems and Quantitative **Biology: Drugs and Small Molecules** Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 4 Laura Jarboe, Co-Chair

Mehmet Orman, Co-Chair Stephanie McCalla, Co-Chair

Sponsored by: Bioengineering

- 12:30 Paper 710a: Metabolic Modeling of Susceptible and Resistant Escherichia coli under Antibiotic Stress
- Sean G. Mack, Eric Hill, Young-Mo Kim, Lye-Meng Markillie, Teresa Palazzo, Robert Young, Karl Weitz, Ganesh Sriram, Daniel J. Dwyer
- 12:48 Paper 710b: Inhibition of Escherichia coli Nitric Oxide Defenses By Amino Acids
- Wen Kang Chou, Mark P. Brynildsen
- 1:06 Paper 710c: Modulation of Chemotaxis By an Interkingdom Signaling Molecule
- Jingyun Yang, Ravi Chawla, Kathy Rhee, Rachit Gupta, Arul Jayaraman, Pushkar Lele
- 1:24 Paper 710d: Network Insights into Improving Drug Target Prediction Accuracy of Inference Algorithms
- Muying Wang, Jason E. Shoemaker
- 1:42 Paper 710e: Metabolomics for Investigating the Effects of Estrogen on **Human Platelets**
- Cara L. Sake, Keith B. Neeves, Nanette R. Boyle
- 2:00 Paper 710f: Cybernetic Modeling of the Inflammatory Response in Mouse Bone Marrow Derived Machrophage
- Lina Aboulmouna, Shakti Gupta, Mano R. Maurya, Shankar Subramaniam, Doraiswami Ramkrishna
- 2:18 Paper 710g: Systems Biology for Biofilm Antibiotic Tolerance
- Philip S. Stewart

(711) Thermoelectric and **Electrochemical Applications of Semiconductors**

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 15 Letian Dou, Chair

Sponsored by: Electronics and **Photonics**

- 12:30 Paper 711a: Panoscopic **Engineering of Nanomaterials** Formodulated Heat Transfer and Beyond — Yue Wu
- 1:00 Paper 711b: Electronic Doping of Semiconductor Thermoelectric Nanostructures with Isoelectronic Dopants
- Ayaskanta Sahu
- 1:30 Paper 711c: Selective CO. Reduction on Isolated Transition Metal Single Atomic Sites: From Identification to Scaling-up
- Haotian Wang
- 2:00 Paper 711d: Phase Diagram Determination of Thermoelectric Aq-Pb-Sn-Te Quaternary System
- Sinn-wen Chen, Yi-Huei Du, Aleš Krouna
- 2:20 Paper 711e: Synthesizing Crystalline Silver Selenide Thin Films for Thermoelectric Applications
- Nan (Louise) Chen, Ayaskanta Sahu

- 2:40 Paper 45b: Nucleation and Growth of Titanium Dioxide Thin Film on Polydimethylsiloxane By Atomic Layer Deposition (ALD)
- **Sarah Hashemi Astaneh**, Gregory Jursich, Cortino Sukotjo, Christos G. Takoudis

(712) Transport Processes in Flow Reactors

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Bayhill 29/30 Haider Al-Rubaye, Chair

Sponsored by: Transport and Energy Processes

12:30 Paper 712a: Diffusion of 1,3,5-Triisopropylbenzene in a Serie of Al₂O₃-Y Zeolite Particles By Zero Length Column Method: From Effective Diffusion to Pore Diffusion Coefficient — *Linxie Hu, Wei Sun, Yuzhi Wei, Zhentao Chen, Suoqi Zhao*

12:50 Paper **712b**: CFD Simulation of Flow and Heat Transfer in Fixed Beds with Axial Thermowells

- Anthony G. Dixon, Yan Wu

1:10 Break

- **1:30 Paper 712d:** Natural Circulation of Single and Binary Gas Mixture in Very High Temperature Reactor
- **Apoorva Rudra**, Masahiro Kawaji
- **1:50 Paper 712e:** Structured Multiphase Reactors for Electrocatalytic CO₂ Conversion
- **J. Ruud van Ommen**, John Nijenhuis, Volkert van Steijn, Johan T. Padding
- **2:10 Paper 712f:** Preparation of Expandable Graphite with a Taylor-Couette Flow Reactor
- **Mohammed AlAmer**, Somayeh Zamani, Yong Lak Joo
- 2:30 Paper 712g: PIV Experimental Characterization of Fluid Dynamics Generated By a Rotating Inner Cylinder with Rough Surface in Taylor—Couette Reactors
- **Bin Li**, Guang Li, Chenyang Xue, Xiaogang Yang

(713) Two-Dimensional Materials

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Celebration 16 Dongxia Liu, Chair Guangwei He, Co-Chair Xueyi Zhang, Co-Chair

Sponsored by: Inorganic Materials

- 12:30 Paper 713a: Enhanced Surface Activity of MWW Zeolite Nanosheets Prepared By a One-Step Synthesis Method
- **Yunwen Zhou**, Ming-Feng Hsieh, Bernd Kabius, Yanyu Mu, Robert Rioux, Jeffrey D. Rimer
- **12:48 Paper 713b:** Vapor-Phase Strategy to Pillaring of Two-Dimensional Zeolite
- Wei Wu**, Dongxia Liu**

- 1:06 Paper 713c: Structural and Catalytic Stability of Aluminosilicate Hierarchically-Structured Two-Dimensional MFI Zeolite Nanosheets Under Steaming
- **Yasmine Guefrachi**, Gaurav Kumar, Katherine P. Vinter, Son-Jong Hwang, Michael Tsapatsis
- **1:24** Paper 713d: Fabrication of AEL Zeolite Nanosheet Membrane on Alumina Hollow Fibers for Molecular-Sieving Applications
- **Akshay Korde**, Byunghyun Min, Shaowei Yang, Aristotle Grosz, Sankar Nair, Christopher Jones
- 1:42 Paper 713e: Efficient Gas Sieving from Assembled Films of Nanoporous Zeolitic and Carbon Nitride Nanosheets
- Mostapha Dakhchoune, Luis Francisco Villalobos, **Kumar Varoon Agrawal**
- 2:00 Paper 713f: Reversible Polycondensation-Termination Growth of 2D Covalent Organic Frameworks with Controlled Morphologies
- Song Wang, **Ziyang Zhang**, Haomiao Zhang, Ananth Govind Rajan, Nan Xu, Yuhao Yang, Yuwen Zeng, Pingwei Liu, Xiaohu Zhang, Qiying Mao, Yi He, Junjie Zhao, Bo-Geng Li, Michael Strano, Wen-Jun Wang
- **2:18 Paper 713g:** Two-Dimensional Organic-Inorganic Hybrid Perovskites Nanomaterials and Heterostructures
- 2:36 Paper 713h: Tunable Interlayer Channels in Graphene Oxide Membranes for Molecular Separations — Shaofei Wang, Suzana P. Nunes

(714) Water Treatment, Desalination, and Reuse II

Thursday, Nov 14, 12:30 PM Hyatt Regency Orlando, Barrel Spring I Ngoc Bui, Co-Chair Oishi Sanyal, Co-Chair Dongmei Li, Co-Chair

Sponsored by: Membrane-Based Separations

- **12:30 Paper 714a:** Functionalized Nanofiltration Membranes for Enhanced Stability in Water Treatment
- Mei-Ling Liu, Dan-Dan Shao, Tian-Dan Lu, Hui-Fang Xiao, Xue-Li Cao, **Shi-Peng Sun**
- **12:52 Paper 714b:** Janus Membranes Via Physicochemical Area Selective Initiated Chemical Vapor Deposition
- **Mahdi Mohammadi Ghaleni**, Mona Bavarian, Siamak Nejati
- 1:14 Paper 714c: Thin Film Nanocomposite Hollow Fiber Membranes Comprising Na+-Functionalized Carbon Quantum Dots for Brackish Water Desalination
- **Wenxiao Gai**, Dieling Zhao, Tai-Shung Chung
- **1:36 Paper 714d:** The Influence of Temperature Gradients on Selective Charge Transport in Electrodialysis Systems
- Anne Benneker

- 1:58 Paper 714e: Thin Film
 Nanocomposite (TFN) Membranes
 Containing Functionalized Zeolite
 Nanoparticles for Desalination with High
 Boron Rejection
- Süer Kürklü-Kocaoğlu, Aysa Güvensoy, Cansu Yildirim, L. Loni Berkel, Cigdem Atalay-Oral, Begüm Tokay, S. Birqül Tantekin-Ersolmaz
- 2:20 Paper 714f: High Concentration Ternary Saline Water Treatment Via Superhydrophobic and Fabricated Antifouling Membrane Via Vacuum Membrane Distillation
- **Yushan Shao**, Yingqi Wang, Gaohong He**, Xiaobin Jiang**
- 2:42 Paper 714g: Membrane
 Degradation of Forward Osmosis (FO)
 in Treating MED Brine: Comparison
 between Cellulose Triacetate (CTA) and
 Thin-Film Composite (TFC) Polyamide
 Membranes
- **Ye Yang**, Yuzhu Sun, Jianguo Yu

(715) Ammonia Energy Implementation Conference: Plenary Session I

Thursday, Nov 14, 1:30 PM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

1:30 Paper 715a: Keynote Speech: Hydrogen and Ammonia: Building Global Momentum — Cedric Philibert

2:00 Panel Discussion

(716) Advanced Inorganic Materials for Membrane Gas Separation

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Coral Spring I/II Xueyi Zhang, Co-Chair Ali Rownagi, Co-Chair Seok-Jhin Kim, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30 Paper 716a:** Highly Permeable Dual-Layer MOF Composite Membranes for Post-Combustion CO₃ Separation
- **Sameh Elsaidi**, Surendar Venna, Mona Mohamed, David Hopkinson
- **3:51 Paper 716b:** Facile and Scalable Fabrication of High-Performance CHA Zeolite Hollow Fiber Membranes and Modules for Gas Separations
- **Shaowei Yang**, Yadong Chiang, Sankar Nair
- **4:12** Paper 716c: Sub-200-Nm Thick Carbon Molecular Sieve Membranes and Modulation of Pore-Size-Distribution By Room Temperature Oxygen Functionalization
- **Shiqi Huang**, Kumar Varoon Agrawal

- **4:33 Paper 716d:** Tuning Carbon Molecular Sieve Hollow Fiber Membranes for Gas Separation through Hyperaging
- Wulin Qiu, Justin T. Vaughn, Gongping Liu, Liren Xu, Mark Brayden, Marcos Martinez, Thomas Fitzgibbonsb, Graham Wenz, William Koros
- **4:54** Paper **716e:** Microporous Inorganic Membranes for Ammonia Separation
- **Surya Padinjarekutt**, Huazheng Li, Ji Jiang, Miao Yu
- **5:15** Paper 716f: Development of Evaluation Method for the Ideal Separation Property of Microporous Membrane: A Case Study for Ag-X Membrane for Propylene/Propane Separation
- **Motomu Sakai**, Naoyuki Fujimaki, Masahiko Matsukata
- **5:36** Paper 716g: Fabrication of Hydrogen-Selective Silicon-Based Ceramic Membranes Via Pyrolysis of Vapor Deposited Polymer Films

 Bryan Nauven, Sasan Dabir.
- **Bryan Nguyen**, Sasan Dabir, Malancha Gupta, Theodore Tsotsis

(717) Advances in Lignin Degradation Strategies

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Discovery 47 Li Shuai, Chair Chang Geun Yoo, Co-Chair

Sponsored by: Forest and Plant Bioproducts Division

- **3:30 Paper 717a:** Oxidative Degradation of Lignin to Value Added Products
- Ajinkya More, Zhihua Jiang
- **3:48** Paper **717b**: Quantitation, Depolymerization, and Demethylation of Lignin in Inorganic Ionic Liquid *Ning Li, Zheng Li, Xuejun Pan*
- **4:06** Paper 717c: Oxidation of Lignin-Rich Residue from Deacetylation, Mechanical Refining, and Enzymatic Hydrolysis of Lignocellulose
- **Jacob S. Kruger**, David Brandner, Camille Amador, Katherine Krouse, Gregg T. Beckham
- **4:24** Paper 717d: Quantum Mechanical Studies of the Depolymerization of Lignin By the ZnCl_z:Ethylene Glycol Deep Eutectic Solvent
- **Alexander Landera**, Lalitendu Das, Anthe George, John M. Gladden
- **4:42** Paper 717e: Non-Catalytic Oxidative Depolymerization of Lignin with Molecular Oxygen to Produce Valuable Phenolic Monomers
- **Parinaz Hafezisefat**, Long Qi, Robert C. Brown
- **5:00** Paper 717f: Lignin Bioconversion: Valorization from Heterogeneous Stream to High-Value Target Compound *Shangxian Xie*

- **5:18** Paper **717g**: Mechanistic Study of Diaryl Ether Bond Cleavage during Lignin Hydrogenolysis Using Advanced Lignin Model Compounds
- **Yanding Li**, Benginur Demir, Steven Karlen, James A. Dumesic, John Ralph
- **5:36 Paper 717h:** Analysis of Pyrolysis Oil Model Compounds Using *in-Situ* raman
- Adhish Madugula, Tracy J. Benson

(718) Biomacromolecular Gels Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Celebration 10 Rachel Letteri, Chair Christina Tang, Co-Chair

Sponsored by: Polymers

- **3:30 Paper 718a:** Antifouling Strategies of Biodegradable Zwitterionic Polyurethane for Implantable Biomedical Applications
- Huifeng Wang, Gang Cheng
- **3:45** Paper **718b**: Characterizing Network Structure in Lignin-Based Hydrogel Composites for Membrane-Based Separations
- **Nicholas Gregorich**, Junhuan Ding, Mark C. Thies, Eric M. Davis
- **4:00** Paper 718c: Collagen-Based Hydrogels for the Encapsulation of Saccharomyces Cerevisiae: Applications in Highly-Efficient Packed-Bed Reactors for Bioethanol Production
- Jorge Luis Patarroyo Argüello, Juan C Cruz, Luis H. Reyes
- **4:15** Paper 718d: Photoresponsive Hydrogel Membranes for High-Throughput Screening and Isolation of Microbes
- **Ryan Hansen**, Tom Platt, Mohammadali Masigol, Niloufar Fattahi, Niloy Barua, Priscila Nieves-Otero, Andre van der Vlies
- **4:30 Paper 718e:** Rheology of Cellulose Nanofibrils in a Viscoelastic Network
- **Ryan Poling-Skutvik**, Chinedum Osuji
- **4:45** Paper **718f**: Anisotropic Chitosan Hydrogels with Multiscale Layered Structures
- Qingye Liu**, Wei Li**
- **5:00** Paper **718g:** Active DNA Olympic Hydrogels Driven By Topoisomerase Activity
- **Brad A. Krajina**, Audrey W. Zhu, Sarah C. Heilshorn, Andrew J Spakowitz
- **5:15** Paper **718h**: Tuning Bulk Hydrogel Degradation By Simultaneous Control of Proteolytic Cleavage Kinetics and Hydrogel Network Architecture
- Christopher M. Madl, Lily M. Katz, Sarah C. Heilshorn
- **5:30** Paper 718i: 4D Patterning of Gel Biomaterials with Bioactive Site-Specifically Modified Proteins
 Jared A. Shadish, Gabrielle M. Benuska, Cole A. DeForest

(719) Biomolecular Engineering Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Celebration 3 Kevin J. Cash. Chair

Kevin J. Cash, Chair Jerome M. Fox, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30 Paper 719a:** Antibody-Enzyme Conjugate Megamolecules with Control of Domain Stoichiometry for Cancer Therapy
- **Kevin Metcalf**, Blaise Kimmel, Justin Modica, Raymond Dai, Zena Werb, Milan Mrksich
- **3:48** Paper **719b**: Design and Characterization of Peptide-Tagged T-Cell Immunoglobulin and Mucin (TIM) for Efficient Recovery of Exosomal Vesicles
- **Yoichi Kumada**, Yuta Atarashi, Junichi Horiuchi
- **4:06** Paper **719c**: An Artificial Golgi Reactor As an Alternative Method for Targeted Cell-Free Glycosylation
- Elli Makrydaki, Ignacio Moya Ramirez, Anja Krueger, Stuart Haslam, Cleo Kontoravdi, Karen Polizzi
- **4:24** Paper 719d: Lipid-Based Drug Delivery Systems Understanding Molecular Packing, Interaction, and Degradation Kinetics and Thermodynamics
- **Ying Liu**, Pin Zhang, Binhua Lin, Wei Bu
- **4:42** Paper **719e**: Non-Porphyrin Photosensitizers for Photodynamic Therapy: Biophysical and Preliminary Cell Studies
- **Poornima Kalyanram, Anju Gupta**, Istvan Stadler
- **5:00 Paper 719f:** The Broad-Spectrum Mechanisms and Design of Capsid Inhibitors for HIV-1
- Alexander J. Pak, Gregory A. Voth
- **5:18** Paper **719g:** Invited: Talking to Cells: Biomolecular Engineering for Non-Invasive Imaging and Control of Cellular Function
- Mikhail G. Shapiro

(720) Catalysis for Biomass Upgrading III: Novel Conversion Strategies

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Florida Ballroom B

George Tsilomelekis, Chair Basudeb Saha, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30 Paper 720a:** Hydrogenolysis of Lignin Model Compounds over Transition Metal Catalysts in a Continuous Flow Reactor
- **Benginur Demir**, Yanding Li, Leida M. Vazquez-Ramos, John Ralph, James A. Dumesic

- **3:48 Paper 720b:** Challenges and Opportunities in the Production of Dimethylfuran from Sugars By Performing Tandem Catalysis
- Sebastian Prodinger, Basudeb Saha, Dionisios G. Vlachos, Raul F. Lobo
- **4:06** Paper **720c:** Catalytic Carbon-Carbon Bond Coupling for Producing Biolubricants from Mixed Organic Acids *Elnaz Jamalzade*, *G. Peter van*
- **Elnaz Jamalzade**, G. Peter van Walsum, Koorosh Kashkooli, Thomas J. Schwartz
- **4:24** Paper 720d: Regio- and Stereo-Selective Synthesis of Hexane-Tetrols and -Triols from Methyl Glycosides over Supported Metal Catalysts
- **Siddarth H. Krishna**, Ji Cao, Masazumi Tamura, Yoshinao Nakagawa, Graeme S. Jacobson, James A. Dumesic, Keiichi Tomishige, George W. Huber
- **4:42** Paper 720e: Mechanism and Kinetics of Ethanol and Acetone Conversion to Isobutene over Zinc Zirconium Mixed Oxide
- **Julie Rorrer**, Alexis T. Bell, Dean Toste
- **5:00** Paper 720f: Effects of Metal Sites on Co-Reactions of Light Alkanes and Biomass-Derived Oxygenates

 Eric Lin, Dante Simonetti
- **5:18 Paper 720g:** Catalytic Production of Renewable Lubricant Base Oils from Biomass
- **Sibao Liu**, Basudeb Saha, Dionisios G. Vlachos
- **5:36 Paper 720h:** Fundamentals of Mechanocatalysis for Lignin Valorization
- Andrew Tricker, George Samaras, Karoline Hebisch, Matthew J. Realff, Carsten Sievers

(721) Catalytic Hydrocarbon Processing III: Fundamentals of Alkane Activation

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom E Sheima J. Khatib, Chair Dante Simonetti, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30 Paper 721a:** Hydrogen and Carbon Nanomaterials Production By Catalytic Decomposition of Methane over Fe and Co Based Catalysts Supported on CeO₂-ZrO₂
- **Vaidheeshwar Ramasubramanian**, Hema Ramsurn, Geoffrey Price
- **3:50 Paper 721b:** Microkinetic Model of Light Olefin Oligomerization on Acidic Zeolites
- **Sergio Vernuccio**, Elizabeth E. Bickel, Rajamani Gounder, Fabio H. Ribeiro, Linda J. Broadbelt
- **4:10 Paper 721c:** Pt Based Bimetallic and Trimetallic Catalysts for Ethane Aromatization
- Junjun Shan

- **4:30** Paper **721d:** Bimetallic Ni/Ga Modified HZSM-5 Catalyst for Ethane Aromatization
- **Siavash Fadaeerayeni**, Yizhi Xiang, Hossein Toghiani, Tingyu Liang
- **4:50** Paper 721e: Insights into the Dehydroaromatization of Ethylene over Ag-ZSM-5 Catalysts Using Transient Kinetics Techniques and Density Functional Theory
- **Hari Thirumalai**, Yunwen Zhou, Unmesh Menon, Jeffrey D. Rimer, Lars C. Grabow
- **5:10** Paper 721f: Insight into the Effects of Ni-Support Interactions on Enhanced Selectivity of Base-Growth CNTs and COx-Free H₂ Production from Thermocatalytic Decomposition of Methane
- Mengze Xu, Libor Kovarik, Stephen Davidson, Juan A. Lopez-Ruiz, Jianli Hu, Robert A. Dagle
- **5:30 Paper 721g:** Dry Reforming of Methane Using Two-Dimensional Vanadium Carbide
- Raj Thakur, Carlos A. Carrero

(722) Cell Migration

Thursday, Nov 14, 3:30 PM
Hyatt Regency Orlando, Celebration 4
Roman Voronov, Chair
Esther Gomez, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30 Paper 722a:** A Novel Microfluidic Platform to Study Galvanotaxis during Confined Cell Migration
- **Soontorn Tuntithavornwat**, Konstantinos Konstantopoulos, Chao Wang
- **3:48 Paper 722b:** Repair of Nuclear Rupture during Cell Migration Requires Barrier-to-Autointegration Factor
- Charles Halfmann, Rhiannon Sears, Aditya Katiyar, London Aman, Qiao Zhang, Christopher O'Bryan, Thomas Angelini, **Tanmay Lele**, Kyle Roux
- **4:06 Paper 722c:** Paving the Way: Migrating Leader Cells Dissociate from Collectively Migrating Sheets Under Geometric Confinement
- **Robert Law**, Nianchao Wang, Zhizhan Gu, Konstantinos Konstantopoulos
- **4:24** Paper **722d**: Biophysical Analysis of Algal Decision Making during Phototactic Movement Using a 3D-Printed Microfluidic Device
- Chrolos O. Sedky, Alexis G. Booe, Jade L. Young, Gabela Nelson, Naohiro Kato, **Adam T. Melvin**
- **4:42** Paper 722e: Cell Sensing and Decision-Making in Confinement: The Role of TRPM_7 in a Tug of War between Hydraulic Pressure and Cross-Sectional Area
- Runchen Zhao, Alexandros Afthinos, Tian Zhu, Panagiotis Mistriotis, Yizeng Li, Selma Serra, Yuqi Zhang, Christopher L. Yankaskas, Miguel Valverde, Sean X. Sun, Konstantinos Konstantopoulos

- **5:00** Paper **722f**: Ranking the Relative Dominance of Migration Cues When Guiding Individual Fibroblasts Faced with a Directional Decision in Simple Microfluidic Bifurcations
- Long Quang Pham, **Anh Tong**, Lydia N. Rodrigues, Yang Zhao, Migle Surblyte, Diomar Ramos, John Brito, Adwik Rahematpura, Roman Voronov
- **5:18** Paper **722g**: Invited: Building the Case for Fiber Curvature: An Essential and Critical Biophysical Cue in Cell Biology
- Amrinder S. Nain

(723) Developments in Alternative Fuels and Enabling Technologies II

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Challenger 38/39

Helen H. Lou, Chair Gaurav Agrawal, Co-Chair Fuyue Stephanie Li, Co-Chair

Sponsored by: Fuels and Petrochemicals Division

- **3:30** Paper 723a: Deployment of Yeast and Enzyme Technologies for Sustainable and Cost-Effective Ethanol Production
- **Panagiotis Sarantinopoulos**, Bert Noordam, Mickel Jansen
- **3:55 Paper 723b:** "Dock and Lock" Covalent Assembly of Designer Cellulosomes
- **Luke F. Bugada**, Paul L. Pushpam, Reid Bailey, Fei Wen
- **4:20 Paper 723c:** Bioethanol Production Using Simultaneous Saccharification and Fermentation (SSF) Technique with Dioscorea Rotundata (Yam) As Raw Material
- Nicolas Sarmiento, Alfredo
 Villadiego, Lilia Carolina Rojas-Pérez,
 Monica Amado
- **4:45** Paper **723d:** Biodiesel Production Using Biopolymer Encapsulated Lipase in Bioreactors
- Jegannathan Kenthorai Raman, **Ravindra Pogaku**
- **5:10** Paper **723e**: Prediction of Yields and Composition of Products from Torrefaction
- **Anna Trubetskaya**, Rory Monaghan, JJ Leahv

(724) Developments in Biorefineries Thursday, Nov 14, 3:30 PM

Hyatt Regency Orlando, Regency Ballroom T

David N. Thompson, Chair Peyman Fasahati, Co-Chair Eric Tan, Co-Chair

Sponsored by: Sustainable Biorefineries

- **3:30** Paper **724a**: Integrated Design, Analysis and Optimization of Chemical Production from Biomass Feedstocks Considering Process and Market Uncertainty
- **Abhay Athaley**, Marianthi lerapetritou

- **3:55** Paper **724b**: Multi-Stream Integrated Biorefinery (MIBR) for Sustainable and Cost-Effective Biofuels and Bioproducts
- Joshua Yuan
- **4:20 Paper 724c:** Valorization of the Organic Fraction of Municipal Solid Waste: Improving Process Efficiency Via Biomass Refining and *in Situ* Electrochemical Separation of Bio Based Products
- **Chrysanthi Pateraki**, Eleni Stylianou, Korneel Rabaey, Apostolis Koutinas
- **4:45 Paper 724d:** Characterization of New Syngas-Fermenting Acetogens for Biofuel Production
- Xiao Sun, **Hasan K. Atiyeh**, Raymond L. Huhnke, Ralph S. Tanner
- **5:10 Paper 724e:** Microbial Fuel Cells for Production of Biopower and Bioproducts
- **Jacob LeBlanc**, Emmanuel Revellame, Gholam Massiha, Dhan Lord Fortela, Wayne Sharp, Shelton Houston
- **5:35 Paper 724f:** Catalytic Steam Gasification of Biomass for Hydrogen Production Using Promoted Ni on g-Alumina Catalysts with Low Loads of Metals: Catalyst Stability and Tar Reduction
- **Benito Serrano Rosales**, Daniel Gibran Gonzalez Castañeda Sr., Adriana Sanchez, Ivan Cruz Reyes, Alan Ruben Calzada Hernandez Sr., Hugo de Lasa, Mario Alberto Gomez Gallardo Jr.

(725) Drug Delivery III

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Celebration 2 Srivatsan Kidambi, Chair Greg Thurber, Co-Chair Natesh Parashurama, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30** Paper **725a**: Efficient Delivery of Nerve Growth Factors to the Central Nervous System for Neural Regeneration
- **Duo Xu**, Yunfeng Lu
- **3:48 Paper 725b:** A Biomimetic Nano-Antidote for Alcohol Intoxication
- **Duo Xu**, Yunfeng Lu
- **4:06** Paper 725c: Computational Modeling for the Comprehensive Drug Release of an Implantable, Bioresorbable Drug Delivery Device *Patrick Giolando, Tamara L. Kinzer*-
- Ursem, Luis Solorio

 4:24 Paper 725d: In Vivo Endothelial
 Untake of Nanoparticles: Impact
- Uptake of Nanoparticles: Impact of Disturbed Flow and Degraded Glycocalyx
- **Nandita Bal**, Ming Cheng, Rajiv Kumar, Srinivas Sridhar, Eno E. Ebong
- **4:42** Break
- **5:00** Paper **725**f: Dual-Responsive Polymersomes As *In Vivo* Enzyme Replacement Therapy to the Brain *Bipin Paruchuri, Sarah Smith, Jessica Larsen*

- **5:18** Paper **725g**: Targeting P-Selectin Using Fucoidan-Doxorubicin Nanoparticles for Effective Metastatic Breast Cancer Therapy
- **Mina Jafari**, Vishnu Sriram, Joo-Youp Lee
- **5:36** Paper **725h:** Targeted Drug Delivery to Atherosclerotic Plaques By VCAM,-Functionalized Liposomal System — *Mahsa Kheradmandi, lan Ackers, Ramiro Malgor, Amir M. Farnoud*

(726) Electrochemical CO₂ Reduction II: Chemicals

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom D Miguel Modestino, Chair Jacob R. Boes, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

3:30 Paper 726a: The e-Refinery: Fossil-Free Production of Base Chemicals

- J. Ruud van Ommen
- **3:48** Paper 726b: Electrochemical Reduction of CO₂ on Cu Catalysts in a Diluted Ionic Liquid/Water Mixture
 Samaneh Sharifi Golru, Elizabeth J. Biddinger
- **4:06** Paper **726c:** PdPt Alloy "Nanoclams" for CO₂ Reduction in Tandem with Microbial Communities to Maximize Faradaic Efficiency to Value-Added Products
- Andrew B. Wong, Joseph Gauthier, Frauke Kracke, Antaeres Antoniuk-Pablant, Karen Chan, Christopher Hahn, Alfred M. Spormann, Thomas F. Jaramillo
- **4:24 Paper 726d:** Sustainable Chemical Production through Two-Step CO₂ Electrolysis
- Matthew Jouny, Feng Jiao
- **4:42 Paper 726e:** Porous Metallic Membranes As High-Performance Cathodes for CO₂ Reduction
- **Gastón O. Larrazábal**, Kevin Zeiter, Sina Baier, Ezra L. Clark, Kasper T. Therkildsen, Ib Chorkendorff, Brian Seger
- **5:00** Paper **726f**: Directing Selectivity of Electrochemical CO₂ Reduction at Plasmonic Cathodes
- **Elizabeth R. Corson**, Erin B. Creel, Ananya Subramani, Davis D. Perez, Robert Kostecki, Jeffrey J. Urban, Bryan D. McCloskey
- **5:18 Paper 726g:** Rational Design of Intermetallic Electrocatalysts for CO Reduction
- **Ezra L Clark**, Degenhart Hochfilzer, Celia S. Cailloux, Gastón O. Larrazábal, Brian Seger, Ib Chorkendorff

- **5:36** Paper 726h: Mechanistic Insights into Electrochemical CO(2) Reduction on Copper and Copper-Based Bimetallic Catalysts
- Hongjie Peng, Michael Tang, Yusaku F. Nishimura, Lei Wang, Stephanie Nitopi, Philomena Schlexer, Michal Bajdich, Carlos Morales Guio, Christopher Hahn, Frank Abild-Pedersen, Thomas F. Jaramillo

(727) Fundamentals of Surface Chemistry II

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Florida Ballroom A Venkat Ravi, Chair Fanglin Che, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30 Paper 727a:** Identification of Catalyst Descriptors for Oxidative Coupling of Methane
- Hakan Demir, Lars C. Grabow
- **3:48 Paper 727b:** Mechanistic Understanding of Redox and Acid Doped Mo₈ V₂Nb₁ Catalysts for Ethane Oxidative Dehydrogenation
- **Michael Royko**, Juan Jimenez, Jochen Lauterbach
- **4:06** Paper 727c: Developing Stability Criteria of Isolated Metal Adatoms on a Well-Defined Copper Oxide Film
- **Nisa Ulumuddin**, Kyle Groden, Alex C. Schilling, E. Charles H. Sykes, Jean-Sabin McEwen
- **4:24** Paper 727d: Synthesis of Supported Bimetallic Nanoparticles Via Surface Inorganometallic Chemistry *Kunlun Ding*
- **4:42** Paper 727e: Transient Kinetic Analysis of Acetone Hydrogenation to Isopropanol over Platinum Catalysts: A Combined Experimental and Theoretical Approach
- **Keishla R. Rivera-Dones**, Benginur Demir, Thomas Kropp, Roberto Schimmenti, George W. Huber, Manos Mavrikakis, James A. Dumesic
- **5:00** Paper 727f: In Situ XAS/SAXS Study of Al₂O₃ Coated Pt-Ga/MgAl₂O₄ Catalysts for Alkane Dehydrogenation *Nadadur Veeraraghavan Srinath*,
- Hilde Poelman, Alessandro Longo, Ji-Yu Feng, Jolien Dendooven, Marie-Françoise Reyniers, Vladimir V. Galvita
- **5:18** Paper 727g: Surface Studies of Functional Alcohol Reactions on Oxygen-Precovered Pt

 Lesli Mark, Naveen Agrawal,

Micheal Janik, J. Will Medlin

- **5:36** Paper **727h:** Spectroscopic Elucidation of Propylene Metathesis Reaction Intermediates Using Modulation Excitation-Phase Sensitive Detection-Diffuse Reflectance
- Techniques

 Bhagyesha Patil, Priya Srinivasan,
 Anand Ramanathan, Amy M. Jystad,
 Marco Caricato, Hongda Zhu, Juan J.
 Bravo-Suarez

(728) Gas Hydrates Science and Engineering: Applications

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Peacock Spring

Amadeu Sum, Chair Praveen Linga, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **3:30** Paper 728a: Techno-Economic Analysis of Clathrate Hydrate Based Desalination (HyDesal) Process Utilizing LNG Cold Energy
- Ponnivalavan Babu, Zheng Rong Chong, Abhishek Nambiar, **Praveen Linga**, Nagu Daraboina
- **3:48** Paper **728b:** Quantifying the Severity of Hydrate Blockage in Systems with Under-Dosed Thermodynamic Inhibitors
- **Temiloluwa O. Kuteyi**, Michael L. Johns, Eric F. May, Zachary M. Aman
- **4:06** Paper **728c:** Efficient Assessment of Gas Hydrate Formation Probability Using the HPS-Alta
- **Peter J. Metaxas**, Vincent W.S. Lim, Paul L. Stanwix, Michael L. Johns, Zachary M. Aman, Eric F. May
- **4:24** Paper 728d: Study of the Thermodynamics and Kinetics of Carbon Dioxide Hydrate Formation and Dissociation
- Kristine Horvat, Stacie Meruelo
- **4:42** Paper **728e:** A Thermodynamic Model to Understand the Gas Exchange Process in CH₄+CO₂ Mixed Gas Hydrates for Methane Gas Production and Carbon Dioxide Sequestration
- **Dnyaneshwar Bhawangirkar**, Jitendra Sangwai
- **5:00 Paper 728f:** Hydrate Based Gas Separation of CH₄-CO₂ gas Mixture in Fixed Bed Reactor
- **Namrata Gaikwad**, Gaurav Bhattacharjee, Omkar Singh Kushwaha, Praveen Linga, Jitendra Sangwai, Rajnish Kumar
- **5:18** Paper **728g**: Phase Equilibrium Prediction for Gas Hydrate: Comparing Equation of State Models
- Harshal J. Dongre, Amiya K. Jana
- **5:36** Paper **728h**: Replacement of CH₄ in the Hydrate By CO₂ and N₂ for Methane Recovery and Carbon Dioxide Sequestration: A Modeling Approach *Dnyaneshwar Bhawangirkar*, *Jitendra Sangwai*

(729) Making Molecular Simulation a Mainstream Chemical Engineering Tool

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Rock Spring I/II Michael R. Shirts, Chair Heather Mayes, Co-Chair

Sponsored by: Computational Molecular Science and Engineering

3:30 Introductory Remarks

- **3:40** Paper **729a**: A Twenty-Five Year Perspective on Differences and Possibilities in the Practical Adoption of Molecular Simulations Vs Computational Quantum Chemistry
- Phillip R. Westmoreland
- **4:00** Paper **729b**: Freud: Powerful Particle Simulation Analysis in Python Vyas Ramasubramani, Bradley Dice, Eric S. Harper, Matthew Spellings, Joshua A. Anderson, Sharon C. Glotzer
- **4:20** Paper 729c: Molecular Simulation and Design Framework (MoSDef) for Transparent, Reproducible, Usable By Others, Extensible Simulations (TRUE)
- Peter T. Cummings, Justin Gilmer, Christoph Klein, Matt Thompson, János Sallai, Andrew Z. Summers, Christopher R. Iacovella, Ákos Lédeczi, Peter Volgyesi, Clare McCabe
- **4:40** Paper **729e**: Large-Scale Nonequilibrium Molecular Simulations of Self-Assembly and Transport Processes
- Michael P. Howard
- **5:00** Paper **729f**: Multirefpredict: An Automated Workflow for Method Selection of First Principles Calculations on Transition Metal Chemistry
- **Fang Liu**, Chenru Duan, Heather J. Kulik
- **5:20 Paper 729g:** Recent Developments in the *Signac* Data Management Framework
- **Bradley Dice**, Carl Simon Adorf, Vyas Ramasubramani, Sharon C. Glotzer

(730) Membrane-Based Organic Solvent Separations II

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Barrel Spring II Ryan Lively, Co-Chair Andrew Livingston, Co-Chair Guanghui Zhu, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30** Paper 730a: Membranes for Continuous, on-Demand Dehydration of Anhydrous Solvents in Flow Chemistry Manufacturing Processes
- **Hannah Murnen**, Christine Parrish, Hank Ludwicki, Robin Featherer
- **3:51 Paper 730b:** Influence of Molecular Interactions, Membrane Swelling and Plasticization on Pure and Mixed Fluid Transport in OSN Membranes
- Kelly Bye, Judy S. Riffle, Michele Galizia
- **4:12 Paper 730c:** Surface-Modified Uio-66-NH₂ Mixed Matrix Membranes for Xylene Isomer Separation
- Matthew Rivera
- **4:33 Paper 730d:** Separation of Vegetable Oil Compounds and Solvent Recovery Using Commercial Organic Solvent Nanofiltration Membranes
- **Gui Min Shi**, Mohammad Hossein Davood Abadi Farahani, Jia Yu Liu, Neal Tai-Shung Chung

- **4:54 Paper 730e:** Design of a Pervaporation Assembly Using Static Mixers
- **Haomiao Zhang**, Agnieszka Ladosz, Klavs F. Jensen
- **5:15** Paper 730f: Organic Solvent Nanofiltration through a Specific Carbonaceous Barrier Containing Interpenetrating Perfluoro-Segments *Antara Priyadarshini, Liang Hong*
- **5:36** Paper 730g: Fabrication of Graphene Oxide (GO) Composite Membranes for Organic Solvent Nanofiltration (OSN)
- **Bofan Li**, Yue Cui, Susilo Japip, Zhiwei Thong, Neal Tai-Shung Chung

(731) Membrane Modeling and Simulation I

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Manatee Spring I

Nils Tilton, Co-Chair Xianghong Qian, Co-Chair Martin Maldovan, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30** Paper 731a: Understanding the Salt Transport Properties of Graphene Oxide Membranes: Permeation Measurements and Electrokinetic Modeling
- **Zhongzhen Wang**, Chen Ma, Meisha L. Shofner, Scott A. Sinquefield, Sankar Nair
- 3:51 Paper 731b: Large-Scale
 Computational Study of Zeolite
 Nanosheets As Pervaporation
 Membranes for Ethanol Extraction
 Changlong Zou, Li-Chiang Lin
- **4:12** Paper 731c: The Effects of Additives on PES Membrane Formation Vis Nips from Dissipative Particle Dynamics Simulations
- **Eric Ledieu**, Suphanat Aphinyan, M. Rosario Cervellere, Paul Millett, David Ford, Xianghong Qian
- **4:33 Paper 731d:** Molecular Dynamics Simulations of Polyamide Water Purification Membranes
- Suwei Liu, Sinan Keten, **Richard M. Lueptow**
- **4:54** Paper 731e: Fast Desalination By Multilayered Covalent Organic Framework (COF) Nanosheets
- Mingjie Wei, Yong Wang, Wei Zhou
- **5:15** Paper 731f: A Molecular Simulation Protocol for Membrane Swelling and Organic Solvent Nanofiltration
- **Jie Liu**, Qisong Xu, Jianwen Jiang
- **5:36** Paper **731g:** Promoted Metallization and Mineralization By Zwitterion Grafting: A Potential Modification of TFC Membranes for Maximized Anti-Fouling Properties Process
- Ming Yi, Yan Wang

(732) Modeling of Fluidization Processes

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Bayhill 19 Azita Ahmadzadeh, Chair Madhusudhan Kodam, Co-Chair

Sponsored by: Fluidization and Fluid-Particle Systems

- **3:30 Paper 732a:** Coarse-Grained DEM for Large-Scale Fluidized Bed Applications
- Nico Jurtz, Oleh Baran, Ravindra Aglave, Ben Freireich, Ray Cocco, Matthias Kraume
- **3:55** Paper 732b: Acquiring DEM Validation Data on an Industrial Scale Casey Q. LaMarche, Steven R. Dahl, Ben Freireich, Ray Cocco, Christine Hrenva
- **4:20** Paper 732c: Evaluating Mixing Performance of a Resonant Acoustic Mixer Both Experimentally and Using a Coupled Lbm-DEM Technique
 Ramon E. Lopez, Joseph J. McCarthy
- **4:45** Paper 732d: Numerical
 Verification and Validation of the Particle
 Tracking Technique in Predicting Particle
 Velocity and Solids Distribution in a
 Travelling Fluidized Bed with CFD-DEM

 Yupeng Xu, Tingwen Li, Sina
 Tehignian Jamal Chanuki Thomas
- Yupeng Xu, Lingwen Li, Sina Tebianian, Jamal Chaouki, Thomas Leadbeater, Rouzben Jafari, David J. Parker, Jonathan P.K. Seville, Naoko Ellis, John R. Grace
- **5:10 Paper 732e:** Cluster Formation Mechanism in Boundless Down-Flow Gas-Particle Systems
- **Noel Gómez**, Alejandro Molina Ochoa, Guy B. Marin, Kevin M. Van Geem
- **5:35** Paper **732f**: Modeling of Complex Liquid-Solid Flow of Particle Swelling in Slurry Loop Reactors
- Ning Yang, Rongtao Zhou

(733) Nanomaterial Applications for Human Health and the Environment Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Regency

Ballroom V Nastassja Lewinski, Chair Yinlun Huang, Co-Chair

Sponsored by: Sustainability Science and Engineering

- **3:30** Paper 733a: Improving Sustainability of CNT/Polymer Composites: Tracking CNTs Release Alexander Orlov, Yue Zhao, David Goodwin, Li Piin Sung, Girish Ramakrishnan, Elijah Petersen
- **3:55 Paper 733b:** Green Solvent for Conjugation of Iron Nanoparticles (Fe₃O₄) and Graphene Oxide (GO) Nanosheets to Remove Water Contaminants
- **Novin Mehrabi**, M.Toufiq Reza, Nirupam Aich

- **4:20** Paper 733c: Continuous in Situ Sensing of Marine Pollutants Using Surface Enhanced Raman Spectroscopy (SERS)
- Timo Küster, Geoffrey D. Bothun
- **4:45 Paper 733d:** Electrocatalysts for the Simultaneous Removal of Nitrate and Ammonia from Wastewater
- **Mohiedin Bagheri Hariri**, Gerardine G. Botte
- **5:10** Paper 733e: Biogenic Metallic Nanoparticles. from Micro-Biofactories to a Nanometric Trojan Horse Approach *David Medina*, *Junjiang Chen*, *Thomas J. Webster*

(734) Nanoscale Phenomena in Macromolecular Systems Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Celebration 5 Matthew D. Green, Chair Joseph F. Stanzione III, Co-Chair

Sponsored by: Polymers

- **3:30 Paper 734a:** Evaluating Corona Stabilization Effects in Thermo-Responsive Polyelectrolyte Complex Micelles
- Sachit Shah, Lorraine Leon
- **3:44** Paper 734b: PSMA-*B*-PNIPAM Copolymer Micelles with Both a Hydrophobic Segment and a Hydrophilic Terminal Group: Synthesis, Micelle Formation and Characterization
- Xiaoyan Zhao, Guorong Shan
- **3:58 Paper 734c:** Block Copolymer Organogels As Potential Payload Delivery Media
- Kenneth Mineart
- **4:12** Paper **734d**: Polymer Bioconjugates: An *in silico* Perspective *Coray M. Colina*
- **4:42** Paper **734e**: Entanglements and Toughness of Model Polymer-Grafted Nanoparticle Monolayers
- **4:56 Paper 734f:** Through-Space Activation of Mechanophores By Rotaxane Molecular Machines

- Jeffrey Ethier, Lisa M. Hall

- **Qiong Wu**, Yunyan Sun, Yun Liu, Jeffrey Moore
- **5:10** Paper **734g**: Light-Responsive Shape Memory Polymer Photonic Crystals Enabled By Photothermal Heating

 Calen Leverant, Can Wang, Pena
- **Calen Leverant**, Can Wang, Peng Jiang
- **5:24** Paper 734h: Hierarchical Assembly of Mixed Nanofillers through Crystallization Induced Ordering

 Andrew Jimenez
- **5:38 Paper 734i:** Multiscale Dynamics in Matrix-Free Polymer Grafted Nanoparticle Systems
- **Mayank Jhalaria**, George Fytas, Brian C. Benicewicz, Sanat K. Kumar
- **5:52** Paper 734j: Combined Numerical and Experimental Study of Shear-Induced Aggregation Using Thermo-Responsive Polymer Nanoparticles

 Jose Francisco Wilson, Miroslav Soos

(735) Nanostructured Biomimetic and Biohybrid Materials and Devices Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Discovery 45 Esmaiel Jabbari, Chair Markita Landry, Co-Chair Gozde Sultan Demirer, Co-Chair

Sponsored by: Bionanotechnology

- **3:30** Paper 735a: Invited Talk: Rapid Prototyping of Biohybrid Nanostructures for Sensing and Responsive Materials *Nigel Reuel*
- **4:00** Paper **735b**: Self-Assembled Hybrid Coiled Coil-DNA Nanostructures *Nicholas Stephanopoulos*
- **4:20** Paper **735c:** Plasmon Induced Photocurrent of Photosystem I Assembled on Metal Nanostructures
- **Ravi Pamu**, Benjamin Lawrie, Bamin Khomami, Dibyendu Mukherjee
- **4:40** Paper 735d: Effect of Di(2-ethylhexyl) Phthalate and Mono(2-ethylhexyl) Phthalate Interactions with a Lipid Membrane
- **Christina M. Bailey-Hytholt**, Tanaya Puranik, Anubhav Tripathi, Anita Shukla
- **5:00** Paper 735e: Rapid Photo-Actuation of a DNA Nanostructure Using an Internal Photocaged Trigger Strand
 Nicholas Stephanopoulos
- **5:20** Paper 735f: Nanoengineering of an Electroconductive Cardiac Patch *Ebrahim Mostafavi*, *Thomas J. Webster*
- **5:40 Paper 735g:** Constrained Growth of Magnetite Nanoparticles Via Artificial Biomineralization
- Allen Eyler, Lorraine Leon

(736) Omics and High-Throughput Technologies

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Celebration 1 Nicholas A. Graham, Chair Nigel Reuel, Co-Chair

Sponsored by: Engineering Fundamentals in Life Science

- **3:30 Paper 736a:** Single Proviral Sequencing of Latent HIV-1 Proviruses Using Droplet Microfluidics
- Chen Sun, Adam Abate
- **3:48** Paper 736b: A Printable Paper-Based Hydrogel Microarray for Drug Screening Enabling Discrimination between True and Promiscuous Enzyme Inhibitors
- Rabia Mateen, Monsur Ali**, Todd R. Hoare**
- **4:06** Paper 736c: Genomics Analysis of Metabolic Pathways of Human Stem Cell-Derived Microglia-like Cells and the Integrated Cortical Spheroids
- **Julie Bejoy**, Yan Li
- **4:24** Paper 736d: Reconstruction of Waddington's Epigenetic Landscape from Single-Cell Transcriptomics of Stem Cell Differentiation
- Nan Papili Gao, **Rudiyanto Gunawan**

- **4:42** Paper 736e: Discovery of Novel Protein Methylation Targets through Unbiased, Global Methyl-Proteomics *Nicolas Hartel, Brandon Chew, Jian Xu, Jian Qin, Nicholas A. Graham*
- **5:00** Paper **736f**: Synglycan: A Glycomics Reporter Toolkit for Multiple Cell Types and *In Vivo* application *Xinheng Yu, Kai Cheng, Gabrielle Pawlowski, Anju Kelkar, Alan Friedman, Shichen Shen, Jun Qu, Sriram*
- **5:18 Paper 736g:** Quantitative Biology with Droplet Microfluidics
- Adam Abate

Neelamegham

(737) Operation of Energy Systems Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Bayhill 24 Mariano Martín, Chair Zukui Li, Co-Chair

Sponsored by: Computers in Operations and Information Processing

- **3:30** Paper 737a: Optimal Scheduling of an Energy System for District Heating *Pedro M. Castro, Lennart Merkert*
- **3:49 Paper 737b:** Distributed Cooperative Industrial Demand Response
- Andrew Allman, Qi Zhang
- **4:08** Paper 737c: Dynamic Performance and Equipment Health Analysis of a Natural Gas Combined Cycle (NGCC) Power Plant for Load-Following Operation
- **Yifan Wang**, Debangsu Bhattacharyya, Richard Turton
- **4:27** Paper 737d: Optimal Design and Operation of Power Plants with Reduced Emissions Via Intermittent Renewable Energy Integration
- **Manali S. Zantye**, M. M. Faruque
- **4:46** Paper 737e: Condition-Based Maintenance and Operation Optimization of Large-Scale Energy Systems
- **Yaqing Wu**, Christos T. Maravelias, Micheal J. Wenzel, Mohammad N. ElBsat, Robert T. Turney
- **5:05 Paper 737f:** Assessment of Frequency Regulation Capacity of Chemical Process Industries
- **Joannah Otashu**, Michael Baldea
- **5:24 Paper 737g:** Bayesian Statistical Learning and Stochastic Programming for Energy Market Participation
- Xian Gao, Alexander W. Dowling
- **5:43** Paper 737h: Superstructure Approach for the Design of Renewable-Based Utility Plants and Cost Estimation of Renewable-Based Steam
- Salvador Pérez Uresti, **Mariano Martín**, Arturo Jiménez-Gutiérrez

(738) Particle Engineering and Design for Product Value Enhancement

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Bayhill 20 Ecevit Bilgili, Chair Pallavi Pawar, Co-Chair

Sponsored by: Particle Production and Characterization

- **3:30** Paper **738a**: Development of Mucous-Penetrating Levodopa-Loaded Microparticles for Treatment of Parkinson's Disease
- Mahasweta Paul, Raymond Lau
- 3:51 Paper 738b: Roles of SDS in Griseofulvin Release from Nanocomposites and Amorphous Solid Dispersions: A Comparative Study Mahbubur Rahman, Faustin Arevalo, Alexander Coelho, Stephanie Ahmad, James Tarabokija, Sayali Bhujbal, Ecevit Bilgili
- **4:12** Paper 738c: Layer-Wise Agglomeration of Urea Granules *Yanjie Chen, Kingsly Ambrose, Dhananjay A. Pai, Carl Wassgren*
- **4:33** Paper 738d: Impact of Dry Coating on Dissolution Profile of Micronized BCS Class II Drugs: Influence of Coating Material Hydrophobicity
 Sangah Kim, Liang Chen, Kuriakose Kunnath, Ecevit Bilqili, Rajesh Davé
- **4:54 Paper 738e:** 3D Printing of Tuneable Coloured Agglomerates Strain Distribution Study of a Single Agglomerate Design
- **Jun Zhang**, Negin Amini, David Morton, Karen Hapgood
- **5:15 Paper 738f:** Interaction of Eugenol and Novel Lignin Grafted Silica Nanoparticles with Synthetic Lipid Bilayers
- **Mahsa Moradipour**, Emily Chase, M. Arif Khan, Shardrack O. Asare, Bert C. Lynn, Stephen E. Rankin, Barbara L. Knutson
- **5:36** Paper 738g: Design of All-Solid-State Lithium-Ion Battery Based on Particle Coating Technology

 — Hideya Nakamura. Risa Sakurai.
- **Hideya Nakamura**, Risa Sakurai, Tomoyuki Masuyama, Shuji Ohsaki, Satoru Watano

(739) Process Design in Energy and Sustainability

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Bayhill 26 Bhavik R. Bakshi, Chair Mona Bavarian, Co-Chair

Sponsored by: Systems and Process Design

- **3:30** Paper 739a: Superstructure Optimization Approach for the Optimization of Biogas Upgrading into Biomethane
- **Edgar Martín-Hernández**, Lidia S. Guerras, Mariano Martín

- **3:49** Paper **739b:** Analysis, Design and Operation of Complex Agriculture Based Process Systems By Programmable Structures
- Monika Varga, Bela Csukas
- **4:08** Paper **739c**: Optimal Process Design for a Sustainable Methanol Production Using Renewable Energies By Applying the Fluxmax Approach
- **Dominik Schack**, Georg S. Liesche, Kai Sundmacher
- **4:27** Paper 739d: A General Evaluation Framework for Direct Nonoxidative Conversion Strategies of Methane to Aromatics
- **Kefeng Huang**, Christos T. Maravelias
- **4:46** Paper 739e: Mathematical Optimization of Membrane-Free Desalination Systems That Utilize Low-Grade Heat
- **Alejandro Garciadiego**, Tengfei Luo, Alexander W. Dowling
- **5:05** Paper **739f**: Optimization-Based Process Design for Demand-Response Market *Particibility*
- **Yu Liu**, Ahmet Palazoglu, Nael H. El-Farra
- **5:24** Paper 739g: Spatially-Explicit Site Design for Sustainable Manufacturing with Ecosystems As Unit Operations
 Michael Charles, Bhavik R. Bakshi
- **5:43** Paper **739h**: A Novel Back-Off Algorithm for Integrating Dynamic Optimization and Scheduling of Batch Processes Under Uncertainty

 Yael Izamal Valdez-Navarro, *Luis A*.
- Ricardez-Sandoval

(740) Process Modeling and Control Applications I

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Bayhill 25 David H. Gay, Chair Ankur Kumar, Co-Chair

Sponsored by: Systems and Process Control

- **3:30** Paper 740a: Model-Based Closed-Loop Controller Design of Multi-Location Vagal Nerve Stimulation for Regulating Cardiovascular System Yuyu Yao, Nitish Thakor, Mayuresh
- **Yuyu Yao**, Nitish Thakor, Mayures. V. Kothare
- **3:49 Paper 740b:** Learning-Based Model Predictive Control for Non-Equilibrium Plasmas
- Angelo D. Bonzanini, Dogan Gidon, David B. Graves, **Ali Mesbah**
- **4:08** Paper **740c**: Optimal Regularization Strategies for Large-Scale Parameter Estimation Problems
- Caroline Satye Martins Nakama, Galo A. C. Le Roux, Victor M. Zavala
- **4:27** Paper 740d: Optimal Start-up of Cryogenic Air Separation Units

 Anthony Quarshie, Christopher L. E. Swartz, Yanan Cao, Jesus Flores-Cerrillo

- 4:46 Paper 740e: Model Predictive
 Control with Real-Time Sustainability
 Monitoring: Application to a
 Nonisothermal and Nonisobaric
 Membrane Reactor for Water-Gas Shift
 Jacob Douglas, Gaurav Mirlekar,
 Shuyun Li, Paul Akula, Fernando V.
 Lima
- **5:05** Paper 740f: Robust Optimal Control of a Novel Process Intensification Strategy for Particulate Manufacturing
- Kanjakha Pal, Zoltan K. Nagy
- **5:24 Paper 740g:** Operational Safety of an Ammonia Process Network Via Model Predictive Control
- **Zhihao Zhang**, David Rincon, Zhe Wu, Carlos Garcia, Panagiotis D. Christofides
- **5:43 Paper 740h:** Meeting Energy Demands in Distributed Pipeline Systems
- Junyao Xie, Stevan Dubljevic

(741) Reaction Engineering for Biomass Conversion

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Plaza International Ballroom F Hsi-Wu Wong, Chair Fernando Resende, Co-Chair M.Toufiq Reza, Co-Chair Hsu Chiang, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **3:30 Paper 741a:** Co-Hydrothermal Liquefaction of Guayule Bagasse and Wastewater Treatment Microalgae
- Feng Cheng, **Rodrigo Rosalez**, Mostafa Dehghanizadeh, Catherine E. Brewer
- **3:51 Paper 741b:** Reaction Condition Optimization of Sorbitol Simultaneous Hydrodeoxygenation over a ReOx-Pd/CeO₂ Catalyst Via Design of Experiments
- **Blake MacQueen**, Jochen Lauterbach
- **4:12** Paper 741c: Adsorption of Biomass-Derived Value-Added Chemicals in a Micro-Packed-Bed Reactor. a CFD Study
- Athanasios Kritikos, Yung Wei Hsiao, Dionisios G. Vlachos, Marianthi Ierapetritou, George Tsilomelekis
- **4:33 Paper 741d:** Elucidating the Effects of ReOx Promoters and Water during Metal-Catalyzed C-O Hydrogenolysis of Alcohols
- **Steven V. Nystrom Jr.**, Manish Godara, Chungta Chen, David Hibbitts
- **4:54** Paper **741e:** Selective Preparation of Pentenoic Acids Via Ring Opening of g-Valerolactone
- Xinlei Huana, Jesse Q. Bond
- **5:15 Paper 741f:** Cold Flow Analysis of a Coal and Biomass Bubbling Fluidized Bed Gasifier
- **Ali Sivri**, Amoolya Lalsare, Cosmin Dumitrescu, Jianli Hu

- **5:36** Paper 741g: The Role of Nickel and Molybdenum Catalysts on the Production of Aviation Fuels from Hydropyrolysis of Biomass
- Devin Chandler, Gabriel Seufitelli, Fernando Resende

(742) Self-Assembly in Solution Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Orlando

Ballroom N
Jinhye Bae, Chair
Alexander Donovan, Co-Chair

Paschalis Alexandridis, Co-Chair Sponsored by: Interfacial Phenomena

- **3:30** Paper **742a**: Self-Assembly of Pluronic Molecules in Water: A Simulation Study with Dissipative Particle Dynamics
- **Daniele Marchisio**, Antonio Buffo, Gianluca Boccardo
- **3:45** Paper **742b**: Molecular Dynamics Study of Choline-Based Ionic Liquids and Water Mixtures
- **Kathryn Piston**, Huilin Ma, Eden E L Tanner, Kelly Ibsen, Samir Mitragotri, Shikha Nangia
- **4:00** Paper **742c**: Modelling External Stimuli on Liquid Crystal Assemblies By Surfactants and Nanoparticles at Nanoscale
- Zeynep Sumer, Alberto Striolo
- **4:15 Paper 742d:** Determining Micelle Lengths and Persistence Lengths from Rheometry
- Grace Tan, Ronald G. Larson
- **4:30** Paper **742e:** Fluorinated Surfactant Micelles: Structure and Interactions in Aqueous Solutions Samhitha Kancharla, Dengpan Dong, Dmitry Bedrov, **Paschalis**

Alexandridis

- **4:45** Paper **742f**: Block Copolymer Micelles Modulated By Ionic Liquids: Thermodynamics and Structure
- Yi Zhang, Zhiqi He, Marina Tsianou, **Paschalis Alexandridis**
- **5:00 Paper 742g:** Polytypism of Close-Packed Block Copolymer Micelles By Temperature Quenching
- **Sangwoo Lee**, Liwen Chen, Hanseung Lee
- **5:15 Paper 742h:** Self-Assembly, Rheology & Dynamics in Biosurfactant/ Surfactant Mixed Systems
- Liangchen Xu, **Samiul Amin**
- **5:30 Paper 742i:** Inhibition of TPX₂ Condensation By Importins
- **Mohammad Safari**, Sabine Petry

(743) Solids Handling: Characterization and Heat Transfer Thursday, Nov 14, 3:30 PM

Hyatt Regency Orlando, Bayhill 21 Emad Abbasi, Chair Maulik Mehta, Co-Chair

Sponsored by: Solids Flow, Handling and Processing

- **3:30 Paper 743a:** Impact of Dry Coating to Improve Bulk Properties of Needle-like Morphology
- **Steven H. Chan**, Joshua Engstrom, Rao Mantri, Kuriakose Kunnath, Rajesh Davé
- **3:51** Paper 743c: The Calibration of DEM Input Parameters for Biomass Using a Cubical Triaxial Tester *Nathaniel Gasteyer*, Hojae Yi, Virendra Puri, Carl Wassgren, Marcial
- Gonzalez
 4:12 Paper 743d: Understanding
 Particle Scale Effect of Mixture
- Segregation

 Kerry Johanson
- **4:33 Paper 743e:** Scale up of Heat Transfer for Dry Granular Material in a Bladed Mixer
- Clara Hartmanshenn, Madeline Halota, Johannes G. Khinast, Charles D. Papageorgiou, Christopher Mitchell, Justin L. Quon, Benjamin J. Glasser
- **4:54** Paper **743f**: Investigating the Influence of Processing Temperature on Powder Flowability
- **Tim Freeman**, Jamie Clayton, Laura Moninaton
- **5:15** Paper 743g: Investigating the Moisture Content Impact on the Flow Behaviour of a Wet Glass Beads Powder Lyes Ait Ali Yahia, Christopher Carmichael, Raffaella Ocone

(744) Sustainability Metrics at the Process and Product Level

Thursday, Nov 14, 3:30 PM
Hyatt Regency Orlando, Blue Spring I/II
Carlos Pozo Fernández, Co-Chair
Larry Erickson, Co-Chair
Yinlun Huang, Co-Chair

Sponsored by: Sustainability

- **3:30 Paper 744a:** Application of Green-Accounting Methods for the Assessment of the Chicago Metropolitan Area's Sustainability Trends
- Bayou Demeke, Andres Argoti
- **3:55 Paper 744g:** Benchmarks and Credentials
- Darlene Schuster
- **4:20 Paper 744c:** Sustainability Metrics for Managing and Processing Food Wastes
- **Moises Gutierrez**, Larry Erickson, Sigifredo Castro, Bin Liu
- **4:45 Paper 744d:** Sustainable Soluble Coffee Production Using Dynamic Membrane Processes
- **Michael Vincent Laurio**, C. Stewart Slater, Mariano J. Savelski
- **5:10 Paper 744e:** Sustainability Assessment: Uncertainty Handling and Impact on Decision Making
- Raha Gerami, Yinlun Huang
- **5:35 Paper 744f:** Statistical Analysis of Streamlined Process Simulation-Based Gate-to-Gate Energy Use for Chemical Reactions and Separations
- **Abhijeet Parvatker**, Matthew J. Eckelman

(745) Sustainable Energy: Generation and Storage

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Regency Ballroom U

Vilas G. Pol, Chair Ashley M. Pennington, Co-Chair Sheila Samsatli, Co-Chair

Sponsored by: Sustainable Energy

- **3:30 Paper 745a:** Optimal Start-up Policies for a Nanofluid Based Solar Thermal Power Plant
- **Angel Omar López-Bautista**, Antonio Flores-Tlacuahuac, K. D. P. Nigam
- **3:45 Paper 745b:** Two-Cell Photoelectrochemical Water Splitting Prototype Demonstration System
- **Avigail Landman**, Avner Rothschild, Gideon S. Grader, Rawan Halabi, Gennady E. Shter, Hen Dotan
- 4:00 Break
- **4:15 Paper 745d:** Iron-Nickel Alloy Films for Neutral Electrolyte Electrochemical Reactions
- **Sergio I. Perez Bakovic**, Prashant Acharya, Lauren F. Greenlee
- **4:30 Paper 745e:** Fresh Look on Wind Power Generation-Upgraded, 25/02/2019
- David Judbarovski

(746) Thermodynamics at the Nanoscale

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Silver Spring

Amish Patel, Chair Nathan A. Mahynski, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **3:30 Paper 746a:** Designer Wetting of Supramolecular Hosts
- Hank S. Ashbauah
- **3:50 Paper 746b:** Role of Interfacial Interactions and Chain Flexibility in Density and Concentration Fluctuations of Layered Polymer Systems
- **Ashwin Ravichandran**, Sriramvignesh Mani, Amish Patel, Rajesh Khare
- **4:10** Paper 746c: [Invited Talk] Quantifying Dynamic Heterogeneity of Glasses: Percolation Perspective
- **David A. Kofke**, Sabry G. Moustafa, Andrew J. Schultz, Francis W. Starr, Jack F. Douglas
- **4:35** Paper **746g**: Modeling Compressibility of Confined Fluids Via Molecular Simulation and Equation of State
- **Christopher D. Dobrzanski**, Nicholas Corrente, Gennady Gor
- **4:55** Paper 746e: [Invited Talk] Colloidal Systems with Both a Short-Range Attraction and Long-Range Repulsion Yun Liu

- **5:20 Paper 746f:** Antagonistic Cooperativity between Antimalarials Controlling b-Hematin Crystallization By Attenuation of Step Pinning
- Peter Vekilov
- **5:40 Paper 746d:** Thermodynamics in Reduced Dimensionalities
- **Kaihang Shi**, J. Matt Mansell, Erik E. Santiso, Keith E. Gubbins

(747) Thermodynamics of Polymers Thursday, Nov 14, 3:30 PM

Hyatt Regency Orlando, Celebration 12/13

Kathleen McEnnis, Chair Jonathan K. Whitmer, Co-Chair

Sponsored by: Polymers

- **3:30 Paper 747a:** Tension-Induced Nematic Phase Separation in Homopolymer Melts
- Wenlin Zhang, Ronald G. Larson
- **3:45** Paper **747b**: Role of Secondary Structure in Protein Liquid-Liquid Phase Separation Highlighted By a New Coarse-Grained Model
- **Nina Jovic**, Gregory L. Dignon, Wenwei Zheng, Young C. Kim, Jeetain Mittal
- **4:00** Paper 747c: Nonsolvent Induced Phase Separation in Films and Droplets
- **Douglas R. Tree**, Dakota Banks, Hayden Hedworth, Timothy R. Scott, Tanner Wilcoxson, Caden B. Wilson
- **4:15** Paper **747d:** Understanding Effect of Viscometric Measurements and Thermodynamic Interactions on Blend Polymer Membranes
- Shubham Lanjewar, Siddhant Waikar, Harshal Marathe, Siddhartha Moulik, Amira Abdelrasoul, Anirban Roy
- **4:30** Paper **747e**: Solvent-Induced Conformation Transition of Bottlebrush Copolymers By Coarse-Grained Molecular Dynamics Simulations
- **Yaxin An**, Samrendra Singh, Sanket Deshmukh
- **4:45** Paper 747f: Fluctuations/ Correlations in Disordered Symmetric Diblock Copolymers: Direct Comparisons between Simulations and Theories
- **Yan Wang**, Delian Yang, Jing Zong, Qiang (David) Wang
- **5:00** Paper **747g**: Understanding the Phase Behavior of Block Copolymers: Incorporating Realistic Complexity into Polymer Simulations
- Jakin B. Delony, Sahar Zenoozi, Peter J. Ludovice, **Clifford L. Henderson**
- **5:15** Paper **747h**: Establishing Structure/Property Interrelations Using Fast Scanning Calorimetry
- Alex Balzer, Allison Brandvold, Brandon Ditullio, Lisa Savagian, Pavel Troshin, Jaime Martin, Natalie Stingelin
- **5:30** Paper **747i**: A Critical Review of Free Volume and Occupied Volume Calculation Methodologies

 Norman Horn

- **5:45 Paper 747j:** Thermodynamic Mixing Rules for Block-Random Copolymers
- Melissa C. Calopiz, John Ste. Marie, Jung Min Kim, Bryan S. Beckingham, **Poornima Padmanabhan**

(748) Water Treatment, Desalination, and Reuse III

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Barrel Spring I Isabel Escobar, Co-Chair William A. Phillip, Co-Chair Mahdi Malmali, Co-Chair

Sponsored by: Membrane-Based Separations

- **3:30** Paper 748a: Novel Thin Film Composite Hollow Fiber Membranes Incorporated with Carbon Quantum Dots for Osmotic Power Generation
- **Wenxiao Gai**, Dieling Zhao, Neal Tai-Shung Chung
- **3:51** Paper 748b: Functionalized High Aspect Ratio PCN-222 Nanoparticles for Tunable Reverse Osmosis Performance Stephen M. Martin, Ethan D. Smith, Amanda J. Morris, Brittany Bonnett
- **4:12** Paper 748c: Arsenate Removal By Reactive Mixed Matrix PVDF Hollow Fiber Membranes with Uio-66 Metal Organic Frameworks
- **Baolin Deng**, Peng Wan, Mengxi Yuan, Xiaolong Yu, Zheng Zhang
- **4:33 Paper 748d:** Functionalized Copper-Metal Organic Framework Ultrafiltration Membrane with Improved Dye Rejection and Flux for Water Treatment
- **Mostafa Dadashi Firouzjaei**, Zane Parkerson, Farhad Akbari Afkhami, Milad R. Esfahani, Arunava Gupta
- **4:54** Paper 748e: Mitigation of Inorganic Fouling on Pressure Retarded Osmosis (PRO) Membranes By Coagulation Pretreatment of the Wastewater Concentrate Feed

 Chun Feng Wan, Chakravarthy S.
- **Chun Feng Wan**, Chakravarthy S Gudipati, Neal Tai-Shung Chung
- **5:15 Paper 748f:** Polyamide/CNT Thin Film Nanocomposite (TFN) RO Membranes with Improved Boron Rejection
- Aysa Guvensoy, Süer Kürklü-Kocaoğlu, Cansu Yildirim, Sadiye Velioglu, **S. Birgül Tantekin-Ersolmaz**
- **5:36** Paper **748g**: Graphene Oxide-Titanium Dioxide Nanohybrids for Designing Nanofiltration Membranes with Enhanced Permeability and Rejection in Dye Desalination
- Novin Mehrabi, Nirupam Aich

(749) Ammonia Energy Implementation Conference: Plenary Session II

Thursday, Nov 14, 3:30 PM Hyatt Regency Orlando, Regency Ballroom P

Sponsored by: Ammonia Energy

- **3:30 Paper 749a:** Keynote Speech: Ammonia Energy Implementation Conference: Green Ammonia Consortium
- Shigeru Muraki
- 4:00 Panel Discussion

(750) Advanced Polymeric Membranes for Gas Separation

Friday, Nov 15, 8:00 AM
Hyatt Regency Orlando, Barrel Spring I
Lingxiang Zhu, Co-Chair
Chen Zhang, Co-Chair
Alexander M. Lopez, Co-Chair

Sponsored by: Membrane-Based Separations

- **8:00** Paper 750a: Facilitated Transport Membranes with Tunable Amine-CO $_2$ Chemistry for Highly Selective $\mathrm{CO}_2/\mathrm{H}_2$ Separation
- Yang Han, W.S. Winston Ho
- **8:21 Paper 750b:** Polymer Genome: An Open Tool for the Polymer Membrane Community
- **Guanghui Zhu**, Anand Chandrasekaran, Chiho Kim, Joshua Everett, Rampi Ramprasad, Ryan Lively
- **8:42** Paper **750c:** The Perfluoropolymer Upper Bound *Albert X. Wu, James A. Drayton, Zachary P. Smith*
- **9:03** Paper **750d**: Polymers with Intrinsic Micro Porosity (PIM-1) Based Compatible Blend Membranes for CO₂ Separation Applications
- Ali Sekizkardes, Samir Budhathoki, Surendar Venna, Victor A. Kusuma, David Hopkinson
- **9:24** Paper 750e: Facile Infusion of Size-Sieving Macrocyclic 3D Cavities into Polymers of Intrinsic Microporosity for Ultra-Efficient Gas Separation and Enhanced Stability Against Aging

 Ji Wu, Susilo Japip, Neal Tai-Shung Chung
- **9:45** Paper 750f: Super-Rigid, Intrinsically Microporous Ladder Polymers for Enhanced Gas Separation Performance and Physical Aging Resistance
- **Tanner Corrado**, Ruilan Guo
- **10:06 Paper 750g:** Microporosity Characterization in Ultra-High Free Volume Glassy Polymers
- **Matteo Minelli**, Ryan Lively, Giulio C. Sarti

(751) Advances in Optimization and Planning

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Celebration 2 Debangsu Bhattacharyya, Chair Xunyuan Yin, Co-Chair

Sponsored by: Computers in Operations and Information Processing

8:00 Paper 751a: Novel Approach to Scheduling of Energy-Efficient Flexible Job Shops

— **Nikolaos Rakovitis**, Nan Zhang, Jie Li, Liping Zhang

- **8:18** Paper **751b**: Delaunay-Based Domain Exploration and Adaptive Placement for Surrogate Based Black-Box Optimisation
- Sushant S Garud, Nivethitha Mariappan**, Iftekhar A. Karimi**
- **8:36** Paper **751c:** Top-Down Approach for Scheduling and Control Under Time-Varying Electricity Prices
- **Gustavo Campos**, Yu Liu, Nael H. El-Farra, Ahmet Palazoglu
- **8:54** Paper 751d: A Novel Two-Stage Stochastic Programming Approach for Batch Processes with Unknown Time of Uncertainty Realization
- **Kavitha Menon**, Ricardo Fukasawa, Luis A. Ricardez-Sandoval
- **9:12** Paper 751e: Economic Model Predictive Control for Closed-Loop Scheduling: Robustness to Disturbances *Robert D. McAllister, James B. Rawlings*
- **9:30 Paper 6iq:** Optimization of 2-EH Product Purification Section Using Advanced Modelling Tools
- Ameen AlGhamdi
- **9:48** Paper **751g:** A Hybrid Framework for Solving Multistage Stochastic Programs Under Both Endogenous and Exogenous Uncertainties
- **Zuo Zeng**, Selen Cremaschi
- **10:06 Paper 751h:** Fairness Measures for Decision-Making and Conflict Resolution
- Apoorva Sampat, Victor M. Zavala

(752) Applied Math for Energy and Environmental Applications

Friday, Nov 15, 8:00 AM
Hyatt Regency Orlando, Celebration 3
Ping He, Chair
Kirti M. Yenkie, Co-Chair
Fernando V. Lima, Co-Chair
Johannes Jäschke, Co-Chair
Gaurav Mirlekar, Co-Chair

Sponsored by: Applied Mathematics and Numerical Analysis

- **8:00** Paper 752a: A Dynamic Genome-Scale Metabolic Network Model for a Novel Methanotroph-Cyanobacteria Coculture
- **Kiumars Badr**, Q. Peter He, Jin Wang
- **8:19 Paper 752b:** Kinetics and Reactor Design for Pyrolytic Treatment of Petroleum-Contaminated Soils
- Ye Gao, Kyriacos Zygourakis
- **8:38 Paper 752c:** Well Placement Optimisation in a Heterogeneous Petroleum Reservoir with Geological Uncertainty
- **Emmanuel I. Epelle**, Dimitrios I. Gerogiorgis
- **8:57 Paper 752d:** Modeling of Thermal Cracking of Natural Gas Liquids: Optimization with Support Vector Machine-Based Constraint Handling Scheme for Stiff ODEs
- **Burcu Beykal**, Melis Onel, Onur Onel, Efstratios N. Pistikopoulos

- **9:16** Paper **752e**: Towards a Novel Energy Price Predictive Framework: The Texas A & M Energy Price Index
- **Stefanos G. Baratsas**, Alexander M. Niziolek, Onur Onel, Logan R. Matthews, Christodoulos A. Floudas, Detlef R. Hallermann, Sorin M. Sorescu, Efstratios N. Pistikopoulos
- **9:35 Paper 752f:** Intensification of Biorefinery Operations Using Building Blocks
- **Srinikhita Vankadari**, Salih E. Demirel, Jianping Li, M. M. Faruque Hasan
- **9:54 Paper 752g:** Hyperbolicity of Heat Transport Processes
- Guilherme Ozorio Cassol Sr., Stevan Dubljevic
- **10:13** Paper **752h:** Constructing Efficient Surrogate Models for High-Dimensional First Principles Systems Under Uncertainty
- **George Makrygiorgos**, Giovanni Maria Maggioni, Ali Mesbah

(753) Data-Driven and Hybrid Modeling for Decision Making Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Celebration 1

Bethany Nicholson, Chair M. M. Faruque Hasan, Co-Chair

Sponsored by: Data and Information Systems

- **8:00** Paper **753a**: A Hybrid Modelling Approach Integrating First Principles Modelling with Subspace Identification
- **Debanjan Ghosh**, Emma Hermonat, Prashant Mhaskar, Spencer Snowling, Rajeev Goel
- **8:19 Paper 753b:** Revisiting Hybrid Modeling: Integrating Machine-Learning Models with Physical Constraints
- William Bradley, Fani Boukouvala
- **8:38 Paper 753c:** A Hybrid Modeling Architecture
- Jacob Hunsberger, Masoud Soroush
- **8:57 Paper 753d:** Data Driven Parameter Reduction
- **Thomas Thiem**, Mahdi Kooshkbaghi, Felix Dietrich**, loannis G. Keyrekidis**
- **9:16** Paper **753e:** Deep Learning Based Hybrid Model of Hydraulic Fracturing Process
- **Mohammed Saad Faizan Bangi**, Abhinav Narasingam, Prashanth Siddhamshetty, Joseph Sang-Il Kwon
- **9:35 Paper 753f:** Randomized Rounding for Best Subset Selection Regression
- Owais Sarwar, Nikolaos V. Sahinidis
- **9:54** Paper 753g: Data-Driven Process Synthesis, Design and Intensification *Akhil Arora*, *Ishan Bajaj*, *M. M. Faruque Hasan*
- **10:13** Paper **753h:** Parameterizations of Data-Driven Process Models for Integrated Stochastic Scheduling and Process Control
- **Jodie Simkoff**, Michael Baldea

(754) Elucidating Catalyst Structures Through Advanced Characterization

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Celebration 16 Tae-Sik Oh, Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper 754a: Raman Spectrokinetics to Gain Insights into the Redox Properties of Supported Vanadium Oxide Catalysts: Surface Structure, Support, and Synergistic Effects
- Jorge Moncada, Carlos A. Carrero
- **8:18** Paper 754b: Molten Salt Hydrates As Solvent Media in the Synthesis of Mesoporous TiO, Flakes
- Trang Tran, Weiqing Zheng, George Tsilomelekis
- **8:36** Paper **754c:** Stanford Synchrotron Radiation Lightsource and the Consortium for Operando and Advanced Catalyst Characterization Via Electronic Spectroscopy and Structure
- **Simon R. Bare**, Adam Hoffman, Alexey Boubnov, Oliver Mueller
- **8:54** Paper **754d:** Time-Resolved Dynamics of Intracrystalline Mesoporosity Generation in USY Zeolite *Aseem Chawla*, *Noemi Linares*, *Javier García-Martínez*, *Jeffrey D. Rimer*
- 9:12 Paper 754e: Computational Modeling of Operando Infrared Spectroscopy for Site-Specific Catalyst Characterization
- **Joshua Lansford**, Dionisios G. Vlachos
- **9:30** Paper **754f**: Rate/Concentration Kinetic Petals for Microkinetic Examination of Catalyst Surface Processes
- Yixiao Wang, M. Ross Kunz, Denis Constales, Gregory S. Yablonsky, **Rebecca Fushimi**
- **9:48** Paper **754g**: *Operando* PM-IRAS for Elucidating Poisoning Mechanisms of Catalytic Membrane Surfaces
- Casey O'Brien
- **10:06** Paper **754h**: In Situ/Operando Gold Plasmon Sensing of Adsorbed Oxygen (O₂-GPS): Activity Trends in CO Oxidation on Supported Gold Catalysts *Priya Srinivasan, Hongda Zhu, Juan J. Bravo-Suarez*

(755) Environmental and Automotive Catalysis I

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Celebration 4 Eleni A. Kyriakidou, Chair Andrea Strzelec, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper 755a: Multi-Functional Catalytic System for NOx Trapping and Hydrocarbon Oxidation from Diesel and Advanced Combustion Engines: Impact of Operating Conditions & Trap Composition
- **Abhay Gupta**, Mushfik Rahman, Sungbong Kang, Unmesh Menon, Lars C. Grabow, Michael Harold
- **8:21 Paper 755b:** Nature of Active Sites for Passive NOx Adsorption on Pd-SSZ-13
- **Bhuiyan Md. Rahman**, Unmesh Menon, Abhay Gupta, Taha Salavatifard, Hari Thirumalai, Michael Harold, Lars C. Grabow
- **8:42** Paper **755c**: High Loadings of Atomically Dispersed Pd in Small-Pore SSZ-13: Superior Low Temperature Passive NOx Adsorber
- Konstantin Khivantsev, Nicholas Jaegers, Libor Kovarik, Feng Gao, **Janos Szanyi**
- **9:03** Paper **755d**: Small Pore Zeolite SSZ-13 Supported Pd As Highly Stable Low-Temperature Methane Combustion Catalysts
- Yanran Cui, Bo Peng, Libor Kovarik, Yong Wang**, Feng Gao**
- **9:24 Paper 755e:** Controlled Synthesis of High Surface Area Pd and Pt/ SiO₂(core)@ZrO₂(shell) Catalysts for Low Temperature Oxidation Applications
- **Chih-Han Liu**, Junjie Chen, Todd J. Toops, Eleni A. Kyriakidou
- **9:45** Break
- **10:06 Paper 755h:** Systematic Identification of Active Site for Propene Combustion Using Pd and Pt Bimetallic Nanocrystal Catalysts
- **An-Chih Yang**, Verena Streibel, Tej S. Choksi, Hassan AlJama, Cody Wrasman, Luke T. Roling, Simon R. Bare, Emmett Goodman, Dionne Thomas, Roel Sanchez, Ansgar Schaefer, Yuejin Li, Frank Abild-Pedersen, Matteo Cargnello

(756) Membrane Modeling and Simulation II

Friday, Nov 15, 8:00 AM
Hyatt Regency Orlando, Barrel Spring II
Xianghong Qian, Co-Chair
Nils Tilton, Co-Chair
Martin Maldovan, Co-Chair

Sponsored by: Membrane-Based Separations

- **8:00** Paper 756a: Modeling of Organic Fouling Based on Interaction between Membrane and Foulants for Reverse Osmosis Membrane
- **Yoshiki Okamoto**, John Lienhard
- **8:21** Paper **756b**: Trade-Off between Selectivities and Permeabilities in Planar Anisotropic Membranes for Gas Separations
- **Juan Manuel Restrepo-Florez**, Martin Maldovan
- **8:42** Paper 756c: Cost Optimization of Pressure Retarded Osmosis

 Alexandra Newby, Timothy Bartholomew, Meagan Mauter

- 9:03 Paper 756d: Rigorous Process Simulation Using Reverse Osmosis (RO) Membrane Unit Operation for Water Desalination
- **James Berthold**, Rasika Nimkar, Prodip Kundu
- **9:24** Paper **756e**: A Novel Methodology to Correctly Compare the Energy Efficiency between Membranes and Distillation
- **Jose Adrian Chavez Velasco**, Mohit Tawarmalani, Rakesh Agrawal
- **9:45** Paper 756f: Chemically Dependent Transport of Small Polar Solutes in a Cross-Linked Hii Phase Lyotropic Liquid Crystal Membrane *Benjamin J. Coscia, Michael R. Shirts*
- **10:06 Paper 756g:** Process Simulation-Based Comparative Study on Selecting Membrane Distillation Configuration M. R. Islam, Chau-Chyun Chen, Mahdi Malmali

(757) Modeling of Lipid Membranes and Membrane Proteins

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Coral Spring I/II Shikha Nangia, Chair Reid C. Van Lehn, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

- **8:00** Paper 757a: Molecular Basis of Glucose Transport Mechanism Via Membrane Transporters in Plants *Diwakar Shukla*
- **8:15** Paper 757b: Elucidating Molecular Mechanisms for Membrane Geometry-Specific Protein Localization
- Mark J. Uline
- **8:30 Paper 757c:** Spatial Distribution of Cholesterol in Symmetric and Asymmetric Lipid Bilayers Studied Using Coarse Grained MD Simulations
- **Mohammadreza Aghaaminiha**, Sumit Sharma
- **8:42 Paper 757d:** Packing, Order, and Interfacial Influences on Permeability through Gel-Phase Lipid Bilayers
- **Alexander Yang**, Christopher R. Iacovella, Michael Thompson, David J. Moore, Clare McCabe
- **8:54 Paper 757e:** Membrane Remodelling By Proteins and Nanostructure
- Amir H. Bahrami, Carol K. Hall
- 9:06 Paper 757f: Kir-Cholesterol Interactions: Molecular Simulations Reveal Cholesterol-Mediated De-Coupling between Functionally Important Domains Essential for Gating — Nicolas Barbera, Irena Levitan, Belinda S. Akna
- **9:18** Paper **757g:** Correlated Membrane Bound Protein Conformational Transitions and Lipid Dynamics Provides New Insights into Leakage Kinetics By Pore Forming Proteins
- Ilanila I. P., **K. G. Ayappa**, Jaydeep Basu

- **9:30** Paper **757h:** Association Patterns of Claudin Proteins Impact the Tight Junction Permeability
- **Nandhini Rajagopal**, Naomi Brandt, Alejandro Durand, Santita Ebangwese, Bailey Felix, Austin Freer, Priya Ganesh, Natalie Petryk, Meishan Wu, Shikha Nanqia
- **9:42** Paper **757i**: All-Atom Molecular Dynamics Simulations of the 5-HT₂B G Protein-Coupled Receptor
- Brandon Peters, Andrew Ferguson
- **9:54 Paper 757j:** Modeling Protein-Lipid Sorting at the HIV-1 Viral Assembly Site
- Viviana Monje-Galvan, Prabuddha Sengupta, Jennifer Lippincott-Schwartz, Jessica M. J. Swanson, Gregory A. Voth
- **10:06 Paper 757k:** Irreversible Thermodynamics of Lipid Membranes: Theory and Computation
- **Amaresh Sahu**, Yannick Omar, Kranthi K. Mandadapu
- **10:18** Paper **757**I: Coarse-Grained Simulations of Alpha-Synuclein Adsorption to Lipid Membranes **Zhizhang Shen**, Brandon Hoover, Regina M. Murphy, Reid C. Van Lehn

(758) Novel Active Phases in Catalyst Design I: Earth Abundant Metals

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Celebration 5 Taejin Kim, Chair Dongting Zhao, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper **758a**: Mesoporous Silicates with Highly Dispersed Molybdenum (Mo-TUD-1) for Enhanced Olefin Metathesis
- **Anoop Uchagawkar**, Anand Ramanathan, Yongfeng Hu, Bala Subramaniam
- **8:18** Paper **758b**: Determining the Thermodynamic Stability of Single-Site Iron Complexes in Nitrogen-Doped Carbon: A Computational Study
- Michael Ayiania, Aidan Garcia, Alyssa Hensley, Kyle Groden, Yong Wang, Manuel Garcia-Perez, **Jean-Sabin McEwen**
- **8:36** Paper **758c:** Rational Design of Single-Site-Based Catalysts for Selective Oxidation of Methane to Methanol
- Oxidation of Methane to Methanol

 Arvin Kakekhani, Allegra A. Latimer,
 Jens K. Nørskov
- **8:54** Paper 758d: Design of Highly Active Cobalt Catalysts for CO₂ Hydrogenation Via the Tailoring of Surface Orientation of Nanostructures

- **Juan Jimenez**, Jochen Lauterbach

9:12 Paper 758e: Complete Methane Combustion over Ni/CexZr₁-XO₂ catalysts — *Junjie Chen, Benjamin Carlson, Jae-Soon Choi, Zhenglong Li, Todd J. Toops, Eleni A. Kyriakidou*

- **9:30** Paper 758f: Ni-MgO Stable and Active Catalysts for the Dry Reforming of Methane Prepared By Paper Assisted Combustion Synthesis
- **Vardan Danghyan**, Alexander Mukasyan, Eduardo E. Wolf
- **9:48** Paper **758g:** Design of Cr-Free Promoted Cu-FeOx Catalysts for High Temperature Water-Gas Shift
- Sagar Sourav, Ozgen Yalcin, Minghui Zhu**, Israel E. Wachs**

10:06 Break

(759) Photocatalysis and Electrocatalysis I

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Celebration 15 Michal Bajdich, Chair Chao Wang, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper **759a**: Hydrogenation of Carbonyl Compounds over Pd in Aqueous Phase Under Charged Conditions: Role of Organic Molecular Structure

 Laura C. Meyer, Udishnu Sanyal,
- Laura C. Meyer, Udishnu Sanyal, Kelsey A. Stoerzinger, Donald M. Camaioni, Oliver Gutiérrez, Johannes A. Lercher
- **8:20 Paper 759b:** Fundamental Insights into Electrochemical Oxidation of Methane over Transition Metals
- **Aditya Prajapati**, Brianna Collins, Jason Goodpaster, Meenesh R. Singh
- **8:40 Paper 759c:** Mechanistic Investigations for Electrocatalytic Oxidation of Furfural
- **Naveen Agrawal**, Li Gong, Alex Roman, Lesli Mark, J. Will Medlin, Adam Holewinski, Michael Janik
- **9:00 Paper 759d:** Electrochemical Epoxidation of Olefin Substrates Using Water As the Oxygen Atom Source
- **Kyoungsuk Jin**, Joseph H. Maalouf, Nikifar Lazouski, Nathan Corbin, Dengtao Yang, Karthish Manthiram
- **9:20** Paper **759e:** Fluffy TiO₂-Coating and Tin Oxide Supported Platinum for Ethanol Electro-Oxidation and Oxygen Reduction
- Ahmed Jasim, Yangchuan Xing
- **9:40** Paper 759f: Fundamental Aspects of Formic Acid Electro-Oxidation on Bimetallic Catalysts
- **Ellen A. Murray**, Ahmed Elnabawy, Manos Mavrikakis
- **10:00** Paper **759g:** Effects of Temperature on the Selectivity of Furfural Hydrogenation and Hydrogenolysis Products over Copper Electrocatalysts
- Andrew S. May, Elizabeth J. Biddinger

(760) Syngas Production and Gas-to-Liquids Technology

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Celebration 6 Hema Ramsurn, Chair Erdem Sasmaz, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

- **8:00** Paper 760a: Investigations of the Wax–Water Interface and Impacts of Water in the Micropores of Fischer-Tropsch Synthesis Catalysts
- **Pavlo Kravchenko**, Nicholas Brunelli, David Hibbitts
- **8:20** Paper 760b: Effects of Mn Promoter in Controlling Geometric and Electric Properties of Fe-Based Catalysts for Syngas-to-Olefins Reaction
- **Zixu Yang**, Zhengpai Zhang, Yitao Liu, Jing Xu, Yi-Fan Han
- **8:40** Paper 760c: Composite Mixed Ionic-Electronic Conducting Materials for Low-Temperature Thermochemical CO₂ Splitting and Syngas Generation
- **Qiongqiong Jiang**, Yunfei Gao, Vasudev Pralhad Haribal, Hui Hong, Fanxing Li, Hongquang Jin
- **9:00** Paper 760d: Reaction Mechanism and Microkinetics of the Cobalt—Catalyzed Fischer—Tropsch Synthesis—G. T. Kasun Kalhara Gunasooriya,
- **9:20 Paper 760e:** Dry Reforming of Methane Using Two-Dimensional Metal Carbides
- **Raj Thakur, Raj Thakur**, Carlos A. Carrero, Justin Smith
- **9:40** Paper 760f: Measurements and Modeling of Pressure Drop and Heat Transfer in ZoneFlowTM Structured Catalytic Reactors for Steam Methane Reforming
- **Florent Minette**, Luis Calamote de Almeida, Juray De Wilde
- **10:00 Paper 760g:** Effect of Mesoporous Silica Support (MCM-41, SBA-15, KIT-6) on Fischer Tropsch Studies Using Co-Ru Bimetallic Catalyst in 3D- Printed Stainless Steel Microreactor
- **Nafeezuddin Mohammad**, Sujoy Bepari, Shyam Aravamudhan, Debasish Kuila

(761) The Industrial Fluid Properties Simulation Challenge

Friday, Nov 15, 8:00 AM Hyatt Regency Orlando, Manatee Spring I

Jonathan Moore, Chair Daniel W. Siderius, Co-Chair

Sponsored by: Computational Molecular Science and Engineering Forum

- **8:00 Paper 761a:** A Brief History of the Industrial Fluid Properties Simulation Challenge
- Jonathan Moore

8:20 Paper 761b: Introduction to the Eleventh Industrial Fluid Properties Simulation Challenge: Temperature-Dependence at High Pressure for the Viscosity of Diphenylethane

- Scott Bair

8:40 Paper 761c: Presentations By the Challenge Entrants

- Jonathan Moore

10:20 Paper 761d: Results of the Eleventh Industrial Fluid Properties Simulation Challenge

- Scott Bair

(762) Environmental and Automotive Catalysis II

Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Celebration 4 Erdem Sasmaz, Chair Ishant Khurana, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 762a: Aqueous Phase Hydrodechlorination of Trichloroethylene Using Pd Supported on Swellable Organically Modified Silica (SOMS): Deactivation Due to Chloride and Sulfur Species

— **Saurabh Ailawar**, Gokhan Celik, Seval Gunduz, Jeffrey T. Miller, Franklin (Feng) Tao, Paul Edmiston, Umit S. Ozkan

12:48 Paper 762b: Density-Dependent Deactivation Mechanism in Supported Catalysts By High-Temperature Decomposition of Particles into Single Atoms

— **Matteo Cargnello**, Emmett Goodman, Aaron Johnston-Peck, Elisabeth Dietze, Cody Wrasman, Adam Hoffman, Frank Abild-Pedersen, Simon R. Bare, Philipp Plessow

1:06 Paper 762c: Remarkable Self-Degradation of Cu/SAPO-34 Selective Catalytic Reduction Catalysts during Storage at Ambient Conditions — Aiyong Wang, Ying Chen, Eric D.

Walter, Nancy M. Washton, Donghai Mei, Tamas Varga, Yilin Wang, Janos Szanyi, Yong Wang, Charles H. F. Peden, **Feng Gao**

1:24 Paper 762d: Core-Shell Pt/Al₂O₃@ Cu/ZSM-5 Catalyst for Selective NH₃ Oxidation: Synthesis, Evaluation, and Optimization

— **Ghosh Rajat**, Michael Harold, Thuy T. Le, Jeffrey D. Rimer, Di Wang

1:42 Paper 762e: Influence of Zeolite Framework on Cu Ion Mobility and the Kinetics of Low Temperature NOX Selective Catalytic Reduction

— Casey B. Jones, John R. Di Iorio, Ishant Khurana, Sichi Li, Eduard Kunkes, Subramanian Prasad, Ahmad Moini, Fabio H. Ribeiro, William F. Schneider, Rajamani Gounder **2:00** Paper 762f: Spectroscopic and Kinetic Responses of Cu-SSZ-13 to SO₂ Exposure and Implications for NOx Selective Catalytic Reduction

— Arthur J. Shih, Ishant Khurana, Hui Li, Juan M. Gonzalez, Ashok Kumar, Christopher Paolucci, Trevor Lardinois, Casey B. Jones, Jonatan D. Albarracin Caballero, Krishna Kamasamudram, Aleksey Yezerets, W. Nicholas Delgass, Jeffrey T. Miller, Aída Luz Villa, William F. Schneider, Rajamani Gounder, Fabio H. Ribeiro

2:18 Paper 762g: Selective Catalytic Reduction (SCR) of NOx By Ethanol over Ag/Al₂O₃: A Mechanistic Study of the Product Distribution with Spaci-MS/FTIR

— Galen B. Fisher, Amin Reihani, Andrew Brown, Patricia de Sousa Pestana, John Hoard

2:36 Paper 762h: Effects of Surface Species and Dispersion in CeO₂ Supported Transition Metal Oxide Catalysts for NO Reduction By CO Reaction

— **Shuhao Zhang**, JaeHa Lee, Do Heui Kim, Taejin Kim

(763) Integrated Product and Process Design

Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Celebration 2 Mariano Martín, Chair Ravendra Singh, Co-Chair

Sponsored by: Systems and Process Design

12:30 Paper **763a**: Design and Operation of Synthetic Fuels Production from Fossil and Renewable Resources

— **C. Doga Demirhan**, William W. Tso, Clara F. Heuberger, Joseph B. Powell, Efstratios N. Pistikopoulos

12:49 Paper **763b:** A COSMO-Based Inverse Machine Learning Application for Mixture Product Design

— Haitao Mao, Lu Wang**, Lei Zhang**, Rafiqul Gani

1:08 Paper 763c: An Integrated Multilevel Approach to the Rational Design of Polymer with Multiple Product and Process Constraints

— **Xiong Zou**, Yang Yang, Haotian Ye, Weixuan Zhu, Hong-guang Dong, Mingshu Bi

1:27 Paper **763d:** Food Product Design: A Hybrid Machine Learning and Mechanistic Modeling Approach

— Xiang Zhang, Teng Zhou, Lei Zhang, Ka Y Fung, Ka Ming Ng

1:46 Paper **763e:** Optimal Process Design for E-Fuel Production: Increasing the Efficiency of OME, Synthesis Using a New Reaction Pathway

— **Jannik Burre**, Dominik Bongartz, Philipp Dürr, Alexander Mitsos

2:05 Paper **763f**: Reactor Network Development and Retrofitting for Polymer Production

— **Yunhan Wen**, Lorenz T. Biegler, Jeff Ferrio, John Weston, Logan Matthews, Nima Nikbin **2:24** Paper 763g: Design of Integrated Monoclonal Antibody Production: Opportunities for Continuous Manufacturing

— **Sara Badī**r, Kozue Okamura, Nozomi Takahashi, Haruku Shirahata, Hirokazu Sugiyama

2:43 Paper 763h: Initial Investigations in General Optimization-Based Design of Materials

- Helen Durand

(764) Inverse Design of Soft Materials

Friday, Nov 15, 12:30 PMHyatt Regency Orlando, Manatee
Spring I

Poornima Padmanabhan, Chair Kathleen McEnnis, Co-Chair

Sponsored by: Thermodynamics and Transport Properties

12:30 Paper 764a: Grand Canonical Inverse Design of Multicomponent Colloidal Assemblies

— **Nathan A. Mahynski**, Evan Pretti, Vincent K. Shen, Jeetain Mittal

12:45 Paper **764b:** Self-Assembly and Phase Behavior of Mixed Patchy Colloids with Any Bonding Site Geometry: Theory and Simulation

— **Yiwei Zhu**, Walter G. Chapman, Artee Bansal

1:00 Paper 764c: A Theoretical Study of Dynamic Governing Equations for Binary Colloidal Systems Combined Bbgky Hierarchy and Maximum Path Information Entropy Principle

— **Teng Zhao**, Shuangliang Zhao, Honglai Liu

1:15 Paper 764d: Inverse Design for Self-Assembly of Materials with Targeted Mechanical Properties

— **Pengji Zhou**, James C. Proctor, Greg van Anders, Sharon C. Glotzer

1:30 Paper 764e: Solid-Solid Phase Transitions in the NaCI-KCI System — Jamshed Anwar, Christian Leitold, Baron Peters

1:45 Paper 764f: Exploring the Limit of Self-Assembly: High-*X* Block Oligomers

— **Zhengyuan Shen**, Leonel Barreda, Qile Chen, Marc A. Hillmyer, Timothy P. Lodge, J. Ilja Siepmann

2:00 Paper 764g: Transferable Multiscale Model for Simulating Self-Assembled Skin Lipid Mixtures

— Parashara Shamaprasad, Timothy C. Moore, Christopher R. Iacovella, Annette L. Bunge, Clare McCabe

(765) Novel Active Phases in Catalyst Design II: Noble Metals Friday, Nov 15, 12:30 PM

Hyatt Regency Orlando, Celebration 5
Michael M. Nigra, Chair
Matteo Cargnello, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper **765a:** Pd/CeO₂ Catalyst Derived from One-Pot Generated Pd@ Ce-Based Metal-Organic Framework for Efficient CO Oxidation

— Yuhan Xu, Shaohua Xie, Lin Hu, Xiaofeng Feng, Jiguang Deng**, Fudong** Liu

12:48 Paper **765b**: Atomically-Dispersed Pd/ZnO for Selective Non-Aerobic Ethanol Dehydrogenation Reaction

— **Mengyao Ouyang**, Sufeng Cao, Mengwei Li, Maria Flytzani-Stephanopoulos

1:06 Paper **765c**: High-Selectivity Synthesis of H₂O₂ from H₂ and O₂ over Palladium-Based Catalysts at Ambient Pressure

— **Pengfei Tian**, Doudou Ding, Yang Sun, Feixiang Tian, Jing Xu, Yi-Fan Han

1:24 Paper **765d:** Structural and Kinetic Study of CO Oxidation on Single Atom Pt/CeO₂

— Yubing Lu, Deepak Kunwar, Hua Guo, Abhaya K. Datye**, Ayman M.** Kurim

1:42 Paper 765e: Low Temperature Dry Reforming of Methane over Pt Promoted NiCe@SiO₂ Multi–Yolk–Shell Nanotube Catalysts

— **Sunkyu Kim**, Jochen Lauterbach, Erdem Sasmaz

2:00 Paper 765f: Platinum Restructuring By Carbon Monoxide and Stabilization As Single Atoms in Metal Matrices

— **Sufeng Cao**, Yilang Liu, Leelavathi Annamalai, Prashant Deshlahra, Maria Flytzani-Stephanopoulos

2:18 Paper 765g: Zeolite Supported Pt/ Ga Catalysts for Highly Efficient Ethane Dehydrogenation to Ethylene

— **Lu-Cun Wang**, Yanhao Dong, Wei Wu, Ju Li, Dong Ding

2:36 Paper 765h: Creating Metal-Oxide Interfaces in Metal Organic Framework for Efficient Methanol Synthesis from CO₂

— Yifeng Zhu, Jián Zheng, Yanran Cui, Katherine Koh, Libor Kovarik, Donald M. Camaioni, John L. Fulton, Johannes A. Lercher, Oliver Gutiérrez

(766) Photocatalysis and Electrocatalysis II

Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Celebration 15 Karthish Manthiram, Chair Yang Yang, Co-Chair

Sponsored by: Catalysis and Reaction Engineering Division

12:30 Paper 766a: Advanced Materials Design for Visible-Light Driven Clean Chemical and Fuel Production

— Yang Yang

12:48 Paper 766b: Recent Insights into Electrocatalytic Reactions Under Exotic Conditions

— **James R. McKone**, Tejal Sawant, Rituja Patil, Evan V. Miu, Dean Miller

- 1:06 Paper 766c: Maximizing the Efficiencies of Metal-Insulator-Semiconductor (MIS) Photoelectrodes By Controlling the Flux of Charge Carriers with Interfacial Design

 Joseph Quinn, John Hemmerling, Sulfa Line.
- **1:24** Paper 766d: DFT Analysis of Amino Acid Functionalization of Hematite for Electroreduction Catalysis *Sharad Maheshwari*, *Michael Janik*
- **1:42 Paper 766e:** Electrochemical Barriers Made Simpler
- **Joseph Gauthier**, Colin Dickens, Jens Nørskov, Karen Chan
- **2:00 Paper 766f:** Surface Characterization of IrOx/SrIrO₃ Water-Splitting Catalysts
- **Micha Ben-Naim**, Michaela Burke Stevens, Kyuho Lee, Melissa Wette, Alexey Boubnov, Yasuyuki Hikita, Apurva Mehta, Simon R. Bare, Drew Higgins, Thomas F. Jaramillo
- 2:18 Paper 766g: Mapping Free Energies to Design Molecular Electrocatalysts on a Computer Srini Ramakrishnan, Robert M. Waymouth, Christopher E. D. Chidsey
- 2:36 Paper 766h: Tuning HER on Nickel Phosphide Using Chemical Pressure: First Principles and Machine Learning
- **Robert B. Wexler**, John Mark P. Martirez, Andrew M. Rappe
- (767) Process Modeling and Control Applications II
- Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Celebration 3 Ankur Kumar, Chair David H. Gay, Co-Chair
- **Sponsored by:** Systems and Process Control
- **12:30** Paper **767a:** Multi-Objective and Dynamic Real-Time Optimization of Supercritical Coal-Fired Power Plant Cycling *Rebecca Kim, Fernando V. Lima*
- 12:49 Paper 767b: Modeling and Optimization of a Moving-Bed Chemical Looping Process for Coal Combustion — Anca Ostace, Chinedu O. Okoli, Andrew Lee, Anthony P. Burgard, David C. Miller, Debangsu Bhattacharyya
- **1:08** Paper **767c:** Optimal Sensor Placement for Agro-Hydrological Systems
- **Soumya Sahoo**, Xunyuan Yin, Jinfeng Liu
- **1:27 Paper 767d:** Advanced Control of Hybrid Column Flotation
- Maryam Azhin, Qi Liu, Vinay Prasad
- **1:46** Paper **767e**: Physics-Based Models for Precision Machining

 Utsav Awasthi, *George M. Bollas*
- **2:05** Paper **767f**: On the State and Output Sensitivity of First-Principles Models
- **Carlos S. Mendez-Blanco**, Leyla Özkan

- 2:24 Paper 767g: An Extended Algorithm of Generalized Linear Model to Cope with Multicollinearity and Nonlinearity
- **Shimpei Kawada**, Manabu Kano
- 2:43 Paper 767h: Open-Loop Optimal Control of Directed Self-Assembly of Colloidal Particles in a Microfluidic Device Baggie W. Nyande, Richard
- (768) Reactions in Near-Critical and Supercritical Fluids

Lakerveld

- Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Celebration 6 M.Toufiq Reza, Chair Wan-Ting (Grace) Chen, Co-Chair Hema Ramsurn, Co-Chair
- **Sponsored by:** Catalysis and Reaction Engineering Division

Madhav Ghanta, Co-Chair

- **12:30 Paper 768a:** Super Critical Transesterification of Fats and Lipids Extracted from Dissolved Air Flotation Solids
- **Christopher L. Kitchens**, Saptarshi Chakraborty, Chinmay Joshi
- **12:47 Paper 768b:** Kinetics of the Ethylene Oligomerization Under Supercritical Fluid Conditions
- **Gabriel Seufitelli**, Fernando Resende
- 1:04 Paper 768c: Effect of Hydrothermal Carbonization Temperature on Acidic and Basic Groups of Hydrochars Produced from Orange Peel and Grape Skin
- **Nepu Saha**, Maurizio Volpe, Luca Fiori, Roberto Volpe, Antonio Messineo, M.Toufiq Reza
- **1:21 Paper 768d:** The Use of Supercritical Water for the Liquefaction of Polypropylene into Oil
- **Wan-Ting (Grace) Chen**, Jin Kai, N. H. Linda Wang
- **1:38** Paper **768e**: Hydrogen Production from Iron Corrosion in CO₂/H₂O High Pressure Media
- **Cyrielle Fauveau**, Anais Cario, Cyril Aymonier, Samuel Marre
- 1:55 Paper 768f: NMR of Chemical Reactions at Elevated Process Conditions
- **Hilary T. Fabich**, Stephen A. Altobelli, Partha Nandi, Hans Thomann, Mark S. Conradi
- 2:12 Paper 768g: Effect of Coke Solubility on Product Yield on the Ethylene Oligomerization Under Supercritical Conditions
- **Gabriel Seufitelli**, Fernando Resende
- (769) Real-Time Optimization of Operations
- Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Celebration 1 Ali Mesbah, Chair Gautam Kumar, Co-Chair
- **Sponsored by:** Computers in Operations and Information Processing

- **12:30** Paper **769a**: A Modifier Adaptation Approach to Real-Time Optimization Employing Machine Learning and Trust-Region Techniques *E. Antonio del Rio Chanona, José Eduardo A. Graciano, Benoit Chachuat*
- **12:49** Paper **769b**: Novel Approaches to Online Process Optimization Under Uncertainty
- **Dinesh Krishnamoorthy**, Sigurd Skogestad
- 1:08 Paper 769c: Online Process
 Optimization Using a Surrogate Optimizer
 Dinesh Krishnamoorthy, Allyne dos
 Santos, Sigurd Skogestad
- **1:27** Paper **769d:** Online Scheduling: Addressing Endogenous Uncertainties *Dhruv Gupta*, *Christos T. Maravelias*
- 1:46 Paper 769e: Optimal Online Batch Process Scheduling: Definition, Computations, and Role of State Estimation in Scheduling
- **Venkatachalam Avadiappan**, Christos T. Maravelias
- **2:05 Paper 769f:** Enhancing Real Time Optimization through Multiparametric Programming
- **Justin Katz**, Efstratios N. Pistikopoulos
- 2:24 Paper 769g: Economic Model
 Predictive Control Base on a DataDriven Input-Output Model

 Yu Yang, Jasper Kelly
- 2:43 Paper 769h: Integration of Scheduling and Control within a Dynamic Real-Time Optimization (DRTO) Framework — Jerome Remigio, Christopher L. E. Swartz
- (770) Thermophysical Properties of Biological Systems
- Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Coral Spring I/II Phanourios Tamamis, Chair Jens Glaser, Co-Chair
- **Sponsored by:** Thermodynamics and Transport Properties
- **12:30** Paper **770a**: Studying RNA Modulated Protein Liquid-Liquid Phase Separation Using Coarse-Grained Models *Roshan M Regy, Gregory L. Dignon, Jeetain Mittal*
- **12:48** Paper 770b: Using Parallel Bias Metadynamics to Efficiently Explore Peptide Folding over a Range of Cytostolic Salinities
- **J. Patrick Brian**, Vance Jaeger
- 1:06 Paper 770c: Atomistic and Coarse-Grained Molecular Dynamics Simulations of Elastin-like Peptides and Collagen-like Peptides
- **Phillip Taylor**, Prhashanna Ammu, Arthi Javaraman
- **1:24** Paper **770d:** Atomistic Simulation and Molecular Field Theory Study of DNA Hybridization in Self-Assembling Monolayer Surfaces
- **Merina Jahan**, Heng Ma, Mark J. Uline, Tao Wei

- **1:42 Paper 770e:** Role of Posttranslational Modifications on Protein-Lipid Interactions
- Nandhini Rajagopal, Shikha Nangia
- 2:00 Paper 770f: Influence of Single-Stranded DNA Coatings on the Interaction between Graphene Nanoflakes and Lipid Bilayers — Timothy C. Moore, Alexander Yang, Oluwalade Ogungbesan, Remco Hartkamp, Chris Iacovella, Qi Zhang, Clare McCabe
- 2:18 Paper 770g: Complexation in Globular Protein and Polyelectrolyte Mixtures: Effect of Charge Regulation and Patchiness
- **Rituparna Samanta**, Venkat Ganesan
- **2:36** Paper 770h: Computational Studies on Amyloid Disassembly Using Molecular Dynamics Simulations and Free Energy Calculations
- **Joseph M. Jakubowski**, Asuka A. Orr, Doan Le, Phanourios Tamamis
- (771) The Science of Catalyst Synthesis and Processing
- Friday, Nov 15, 12:30 PM Hyatt Regency Orlando, Celebration 16 Xueyi Zhang, Chair Tej S. Choksi, Co-Chair
- **Sponsored by:** Catalysis and Reaction Engineering Division
- **12:30 Paper 771a:** Synthesis Gas Conversion over Rh/Mo Catalysts
- Prepared By Atomic Layer Deposition
 Lifeng Zhang, Madelyn R Ball, Yifei
 Liu, Thomas F. Kuech, George W. Huber,
 Manos Mavrikakis, Ive Hermans, James
 A. Dumesic
- 12:48 Paper 771b: Switchable Surfactants for the Preparation of Monodisperse, Surface-Clean Supported Nanoparticle Catalysts and the Impacts of Calcination
- Kristin Bryant, Steven R. Saunders
- **1:06** Paper **771c**: Strong Electrostatic Adsorption for the Facile Synthesis of Supported, Dilute Limit Alloy Nanoparticles
- **Leandro T. De Castro**, John R. Regalbuto
- 1:24 Paper 771d: Development of Continuous Co-Electroless Deposition and Improvements Made to Catalyst Activity and Stability
- **Gregory L. Tate**, Bahareh Alsadat Tavakoli Mehrabadi, Wen Xiong, Fahim Rahman, Benjamin H. Meekins, Weijian Diao, John R. Monnier
- 1:42 Paper 771e: Porous Polymer/ Nanocrystal Composites with Wide Tunability and Shape-Selective Catalysis — Andrew Riscoe, Cody Wrasman, Aditya Menon, Larissa Kunz, An-Chih Yang, Matteo Cargnello
- 2:00 Paper 771f: Improving Thermal Stability of Supported Metal Catalysts Via Phosphonic Acid Self-Assembled Monolayers
- **Alexander H. Jenkins**, Charles B. Musgrave, J. Will Medlin

2:18 Paper 771g: Insights on the Thermal Stability of V₂CTx Mxene Under Different Environments

— **Raj Thakur**, Carlos Carrero

2:36 Paper 771h: Correlating Treatment Conditions and Atomic-Scale Environments of Pt Supported on NaY Zeolite
— Tsatsral Battsengel, Bradley F.
Chmelka

(772) Overview of Hydrogen and Fuel Cell Technologies

Tuesday, Nov 12, 8:00 AM Hyatt Regency Orlando, Regency Ballroom O

Sponsored by: Center for Hydrogen Safety

(773) Practicing Hydrogen Safety for Students and Researchers

Tuesday, Nov 12, 9:10 AM Hyatt Regency Orlando, Regency Ballroom O

Sponsored by: Center for Hydrogen Safety

(775) AIChE K-12 STEM Showcase & STEM Outreach Competition

Sunday, Nov 10, 12:30 PM

Hyatt Regency Orlando, Regency Ballroom U

Sponsored by: Miscellaneous

(781) The National Academies of Sciences, Engineering, and Medicine Town Hall: Chemical Engineering in the 21st Century

Wednesday, Nov 13, 8:00 AM Hyatt Regency Orlando, Florida Ballroom C

Sponsored by: Miscellaneous



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Attend the many events and sessions focusing on the positive societal impact made by chemical engineers **#Allforgood**

All for Good: Engineering for Inclusion

A core priority of the Doing a World of Good campaign Increasing inclusion at every stage of the career continuum

Saturday, November 9

LGBTQ+ & Allies Student Ice Cream Social 4:30 PM - 5:30 PM (Annual Student Conference)

Sunday, November 10

AIChE K-12 STEM Showcase 9:15 AM - 2:45 PM

Disability OutReach Inclusion Community (DORIC) ChemE Students with Disabilities & Allies: Expanding **Opportunities and Creating Communities** 2:00 PM - 3:30 PM (Annual Student Conference)

Monday, November 11

Unconscious Bias in Engineering Workshop 8:00 AM - 11:00 AM

Women in Chemical Engineering (WIC) **Networking Luncheon (Ticketed Event)** 11:00 AM - 12:30 PM

Minority Affairs Committee (MAC) **Eminent Engineers Awards Ceremony** With Poster Session 5:30 PM - 7:00 PM

Minority Affairs Committee (MAC) Reception 7:00 PM - 9:00 PM

Tuesday, November 12

The Current State of STEM Inclusion in the Workplace 2:00 PM - 3:00 PM

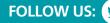
LGBTQ+ & Allies Inclusion in Engineering 3:30 PM - 6:00 PM

LGBTQ+ & Allies Reception 6:15 PM - 7:15 PM















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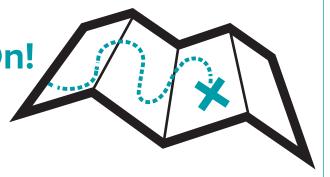
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HONORING

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Chairman and Chief Executive Officer Merck & Co., Inc.

DAVID S. TAYLOR

Chairman, President and Chief Executive Officer
The Procter & Gamble Company

SPECIAL FEATURE

"Doing a World of Good" Medal will be presented to

JAY D. KEASLING

Professor, University of California, Berkeley and Senior Faculty Scientist, Lawrence Berkeley National Laboratory



Recognizing Companies and Leaders Advancing Chemical Engineering while Addressing Societal Needs

TUESDAY, DECEMBER 3

GRAND HYATT NEW YORK, 109 E 42ND STREET, NEW YORK CITY

RESERVE YOUR SEAT

aiche.org/galareservations

2019 ANNUAL MEETING CODE OF ETHICS

Members of the American Institute of Chemical Engineers shall uphold and advance the integrity, honor and dignity of the engineering profession by:

- Being honest and impartial and serving with fidelity their employers, their clients, and the public;
- Striving to increase the competence and prestige of the engineering profession;
- Using their knowledge and skill for the enhancement of human welfare.

TO ACHIEVE THESE GOALS, MEMBERS SHALL:

- Hold paramount the safety, health and welfare of the public and protect the environment in performance of their professional duties.
- Formally advise their employers or clients (and consider further disclosure, if warranted) if they perceive that a consequence of their duties will adversely affect the present or future health or safety of their colleagues or the public.
 - Accept responsibility for their actions, seek and heed critical review of their work and offer objective criticism of the work of others.
 - Issue statements or present information only in an objective and truthful manner.
 - Act in professional matters for each employer or client as faithful agents or trustees, avoiding conflicts of interest and never breaching confidentiality.
 - Treat fairly and respectfully all colleagues and co-workers, recognizing their unique contributions and capabilities.
 - Perform professional services only in areas of their competence.
 - Build their professional reputations on the merits of their services.
 - Continue their professional development throughout their careers, and provide opportunities for the professional development of those under their supervision.
 - Never tolerate harassment.
 - Conduct themselves in a fair, honorable and respectful manner.

SEXUAL HARASSMENT TRAINING

Mandatory sexual harassment training for all Board members, Operating Council Chairs and full-time AlChE Staff members is required by AlChE. The training program is coordinated by AlChE's Human Resources Department. For more information on this topic, please contact **humanresources@aiche.org**.

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Choose Your Own Adventure

Finish 2019 with these exciting conferences and workshops!

Choose your adventure and attend a conference in a new place, participate in a symposium on cuttingedge topics and meet like-minded professionals from around the world.

Polymers and Textiles Conference

November 6-8 | Lowell, MA

2019 AIChE Annual Student Conference

November 8-11 | Orlando, FL

Industrial Water Use and Reuse Workshop

November 9-10 | Orlando, FL

Conference on Engineering Cosmetics and Consumer Products (ECCP)

November 9-10 | Orlando, FL

2019 AIChE Annual Meeting

November 10-15 | Orlando, FL

2nd Space Travel: Adaptive Research and Technologies from Biological and Chemical Engineering (STAR Tech)

November 18-20 | Boston, MA

PD2M Future of Pharmaceutical Manufacturing Workshop

November 21-22 | Washington D.C.

2nd International Conference on Microbiome Engineering

December 2-4 | Boston, MA

2019 AIChE Annual Gala

December 3 | New York, NY

Cell Free Systems Conference

December 4-6 | Boston, MA

2019 Food Innovation and Engineering (FOODIE)

Asia Conference

December 5-6 | Singapore

Food-Energy-Water Nexus

December 5-6 | New York, NY

2019 Food Innovation and Engineering (FOODIE) Conference

December 8-10 | Philadelphia, PA

Optogenetic Technologies and Applications

December 8-10 | Boston, MA

7th International Conference on Stem Cell

Engineering 2019

December 11-13 | Barcelona, Spain

Engineering Sustainable Development

December 12-13 | Seoul, South Korea

Solar Energy Systems Conference

December 12-13 | Waco, TX

Sustainable Packaging Symposium

December 16-18 | Santa Barbara, CA



Choose your adventure: aiche.org/events2019

Event details including dates and locations are subject to change, please check website for most current information.













SAVE THE DATE

AIChE® ANNUAL MEETING | NOVEMBER 15 -20, 2020 | SAN FRANCISCO, CA

The Increasing Diversity of Chemical Engineering

Diversity and inclusion is absolutely necessary to effectively compete in a globalized world. The 2020 AIChE Annual Meeting will feature programming in the area of diversity and inclusion in both academia and industry to help reach diversity goals throughout chemical engineering.

FEATURED SESSION

MEET THE LEADERS: ENGINEERING FOR INCLUSION Tuesday, November 17 | 11:00 AM - 12:30 PM

This plenary session will focus on ongoing success stories in diversity and inclusion and feature a moderated panel of executives from industry and senior academic administrators.



MEETING CHAIRS



Jennifer Sinclair Curtis
Distinguished Professor of
Chemical Engineering
Dean of the College of Engineering
University of California, Davis

PROGRAM CHAIR

PROGRAM CO-CHAIR



Isabel Escobar
Professor of Chemical & Materials
Engineering
University of Kentucky



Jamie Hestekin Professor, Ralph E. Martin Professorship in Chemical Engineering University of Arkansas

PROGRAM CO-CHAIR

SEE YOU IN SAN FRANCISCO!

